"Multiscale modeling of the damage and failure of homogeneous and short-fiber reinforced thermoplastics under monotonic and fatigue loadings"

Krairi, Anouar

ABSTRACT

Reinforced and unreinforced thermoplastic polymers (TPs) are widely used in a range of industrial sectors such as in automotive, aerospace, sporting goods, consumer electronics, and many other domains, because of their interesting properties and their relatively ease of production. Their behavior is rather complex as it is time, strain rate and temperature dependent and couples both viscoelastic and viscoplastic modes of deformation. As a result of their important expansion, produced parts are more likely to be subjected to extreme operating conditions such as fatigue, or exposed to aggressive environments. The effect of these demanding conditions is reflected in a degradation of the material's mechanical properties throughout its lifetime, which is usually the cause of material failure. Hence numerical prediction tools for damage and failure are required, in order to obtain reliable estimates of the material response. The aim of this thesis is to numerically predict the damage and...

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Multiscale modeling of the damage and failure of homogeneous and short-fiber reinforced thermoplastics under monotonic and fatigue loadings

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Thesis submitted in fulfillment of the requirements for the Ph.D. Degree in Engineering Sciences

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Pr. T. Pardoen, Chairman (Université catholique de Louvain, Belgium)
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Abstract

Reinforced and unreinforced thermoplastic polymers (TPs) are widely used in a range of industrial sectors such as in automotive, aerospace, sporting goods, consumer electronics, and many other domains, because of their interesting properties and their relatively ease of production. Their behavior is rather complex as it is time, strain rate and temperature dependent and couples both viscoelastic and viscoplastic modes of deformation. As a result of their important expansion, produced parts are more likely to be subjected to extreme operating conditions such as fatigue, or exposed to aggressive environments. The effect of these demanding conditions is reflected in a degradation of the material’s mechanical properties throughout its lifetime, which is usually the cause of material failure. Hence numerical prediction tools for damage and failure are required, in order to obtain reliable estimates of the material response.

The aim of this thesis is to numerically predict the damage and failure of both thermoplastic polymers (TPs) and misaligned short fiber reinforced thermoplastic polymers (SFRTPs), considered as heterogeneous materials mainly under mechanical fatigue loading with large number of cycles: high cycle fatigue (HCF). The modeling approaches take into account multiaxial stresses and the microstructure of the studied materials. To predict the effective response of the studied heterogeneous materials from their microstructure, multiscale approaches were employed. These approaches represent the modern way of modeling materials because they enable to understand, quantify and optimize the relationship between the final properties of a material or a part at the macroscopic scale and the microstructure.

In the first part of this thesis, the focus is on the modeling of the behavior of unreinforced TPs, motivated by experimental observations showing the important role of the TP matrix in the behavior of the SFRTPs. The modeling approaches take into account the viscoelasticity coupled with viscoplasticity, was developed for homogenous TP materials. A key concept in the proposed approaches is that the damage and defects, causing TPs and SFRTPs failure under HCF, are localized at limited zones within the material, in agreement with experimental findings. Mean field homogenization techniques were developed and employed in order to take into account localized fatigue damage zones, the latter are modeled by so-called "weak spots", which are assumed to have a viscoelastic viscoplastic damaged behavior. The results of the different proposed modeling approaches were validated against available
experimental results. For unreinforced TPs, the experimental data were collected from the open literature. However, for the SFRTPs, our partners in the EUREKA/DURAFIP project which aims at the lifetime investigation of short-glass fiber reinforced Polyamide 66, provided the experimental results of monotonic and fatigue tests.
Abbreviations

CDM  Continuum damage mechanics
FE   Finite Element
HCF  High cycle fatigue
MFH  Mean field homogenization
GF   Glass fiber
HDPE High-density polyethylene
PA66 Polyamide 66
PP   Polypropylene
SFRT(s) Short fiber reinforced thermoplastic polymer(s)
SGFRPA66 Short glass fiber reinforced Polyamide 66
TP(s)  Thermoplastic polymer(s)
E    Elastic(ity)
EP   Elasto-plastic(ity)
EVP  Elasto-viscoplastic(ity)
VE   Viscoelastic(ity)
VEVP Viscoelastic(ity)-Viscoplastic(ity)
VEVPD Viscoelastic(ity)-Viscoplastic(ity)-Damage(d)
VP   Viscoplastic(ity)
PG(s) Pseudo-grain(s)
RVE  Representative volume element
WS(s) Weak-spot(s)
LCC  Linear comparison composite
<table>
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<tr>
<td>MT</td>
<td>Mori-Tanaka</td>
</tr>
<tr>
<td>SC</td>
<td>Self-consistent</td>
</tr>
<tr>
<td>VT</td>
<td>Voight</td>
</tr>
<tr>
<td>DAM</td>
<td>Dry as-molded</td>
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<tr>
<td>FLD</td>
<td>Fiber length distribution</td>
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<tr>
<td>MFD</td>
<td>Main flow direction</td>
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<tr>
<td>RT</td>
<td>Room temperature</td>
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<tr>
<td>w.r.t.</td>
<td>with respect to</td>
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Notations

Scalars are denoted by regular (not boldface) characters

\[ \alpha \beta \gamma \delta \varepsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega \Gamma \Theta \Lambda \Xi \Omega \Psi \]

Vectors are written in boldface lowercase

\[ \mathbf{abcdefghijklmnopqrstuvwxyz} \]

Second-order tensors correspond to boldface capitals

\[ \mathbf{ABCDEFGHIJKLMNOPQRSTUVWXYZ} \]

\[ I : \text{Identity tensor} \]

Fourth-order tensors:

\[ \mathcal{E} : \text{Symmetric identity tensor, } \mathcal{I}^{\text{dev}} : \text{Deviatoric operator, } \mathcal{I}^{\text{col}} : \text{Spherical operator} \]

Mathematical operators:

| \text{tr}(\cdot) | \text{Trace} |
| \text{det}(\cdot) | \text{Determinant} |
| \delta_{ij} | \text{Kronecker’s symbol} |
| \cdot | \text{Contraction over two indices } \mathbf{A} : \mathbf{B} = A_{ij}B_{ji}; (\mathbf{C} : \mathbf{A})_{ij} = C_{ijkl}A_{lk}, |
| \otimes | \text{Tensorial product } (\mathbf{A} \otimes \mathbf{B})_{ijkl} = A_{ij}B_{kl}, |

Principal invariants of strain and stress, represented by a second order symmetric tensor \( \mathbf{A} \):

\[ I_1 = \text{tr}(\mathbf{A}); I_2 = \frac{1}{2} \left[ I_1^2 - \text{tr}(\mathbf{A}^2) \right]; I_3 = \text{det}(\mathbf{A}) \]

Principal deviatoric invariants for stress tensor \( \mathbf{\sigma} \) are:

\[ J_2 = \frac{1}{2} (s : s); J_3 = \text{det}(s) \]

with \( s = \mathbf{\sigma} - \frac{\text{tr}(\mathbf{\sigma})}{3} \mathbf{I} \) is the deviatoric part of \( \mathbf{\sigma} \)
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Chapter 1

Introduction

This chapter serves as an introduction to the present work. A selection of experimental observations about the studied materials is analyzed, in order to motivate the proposed modeling approaches. The thesis scope and the report synopsis are detailed, and a list of publications related to this work is given.

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1.1 Work motivations

New materials or generally called advanced materials have been used for several decades, as an alternative for classical materials. So far, their use has been hampered by the lack of predictive numerical simulation tools, especially for failure and lifetime estimation. Among these new materials, reinforced and unreinforced thermoplastic polymers (TPs) are widely used in a range of industrial sectors such as in automotive, aerospace, sporting goods, consumer electronics, and many other domains, because of their interesting physical properties and the relative ease of their manufacturing. Approximately, thermoplastics represent 90% by weight of all plastics consumed world-wide (Biron, 2012). They have been used to accomplish various objectives, among them designing light-weight structures with controlled cost in order to reduce carbon dioxide (CO\textsubscript{2}) emission, which is a major issue in almost all industries. For instance, European automakers are obliged to ensure a reduction of CO\textsubscript{2} emission from their new cars and light commercial vehicles of 30% by 2020, compared to the emission in 2011 (European commission: press release, 2012). As a result of their important expansion, produced parts are more and more likely to be subjected to extreme operating conditions such as thermo-mechanical fatigue, or exposed to aggressive environments. The effect of these demanding conditions is reflected in a degradation of material’s mechanical properties throughout its lifetime, which is a major cause of material failure. Hence numerical prediction tools for reliable estimates of damage and failure are required.

Short fiber reinforced polymers with fiber length less than 1 mm, are known to be suitable to processing and reprocessing compared to the continuous fiber reinforced polymers and long fiber reinforced composites (Mortazavian and Fatemi, 2014), which helps explain their important expansion especially in automotive industry. The combination of a polymer matrix and the fibers, in particular glass fibers, gives interesting mechanical properties, namely in terms of strength and volume weight as depicted in figure 1.1.1.

Monotonic loading at various loading (strain or stress) rates, and fatigue loadings in order to estimate a part’s lifetime, are two of the most challenging loading types for design. Effects of these two loading cases are very often evaluated by costly and time-consuming experiments. Numerical modeling showed an increasing efficiency and allowed to limit recourse to experiments.

In this work, some modeling approaches are proposed for unreinforced and short fiber reinforced TPs. The proposed model for SFRTPs is applied to the material studied in the DURAFIP (“DURabilité des Polyamides Renforcées de Fibres”) project framework, which is short glass fiber reinforced Polyamide 66 (SGFRPA.66) under fatigue loading. The project is a collaboration of fourteen industrial and academic partners:

- **Industrial Partners:** International chemical group SOLVAY, TOYOTA, PSA Peugeot Citroën, TRELLEBORG, SOGEFI-Filtrauto, PROMOLD, ADI, AXS Ingénierie, e-Xstream engineering.

- **Academic Partners:** ENSTA (“École nationale supérieure de techniques avancées”) Bretagne, CEMEF (“Centre de mise en forme des matériaux”)– MINES ParisTech, ENSAM ("École Nationale Supérieure
1.2 Experimental observations of the studied materials

d’Arts et Métiers”), LMGC ("Laboratoire de Mécanique et Génie Civil")
Montpellier, UCL ("Université Catholique de Louvain").

Figure 1.1.1: Strength as a function of density, highlighting the advantages of
using polymers and polymer based composites (Software CES Selector (2011)).

1.2 Experimental observations of the studied materials

In this section, a literature review on experimental works on failure of unrein-
forced thermoplastics (TPs) and short fiber reinforced thermoplastics (SFRTPs)
is presented. This review is needed in order to understand the behavior of the
studied materials and motivate the proposed modeling approaches. The behav-
ior of unreinforced and reinforced TPs shows several similarities, as it will be
detailed in the text, namely because of the viscous behavior of TPs. Although
many experimental studies on TPs and SFRTPs were realized, the current
knowledge about the studied materials is limited, especially compared to the
knowledge of metals. The following subsections summarize the main tendencies
of the studied materials, based on available experimental investigations.

For fatigue testing, the different terms used in order to characterize applied
fatigue loadings are presented in the following. The loading is defined by the
stress amplitude ($\sigma_{\text{amp}}$), the mean stress ($\sigma_{\text{mean}}$) and the loading ratio ($R$),
which are expressed as functions of maximum and minimum stresses ($\sigma_{\text{max}}$
and $\sigma_{\text{min}}$) by:

$$
\sigma_{\text{amp}} = \frac{\sigma_{\text{max}} - \sigma_{\text{min}}}{2}, \quad \sigma_{\text{mean}} = \frac{\sigma_{\text{max}} + \sigma_{\text{min}}}{2}, \quad R = \frac{\sigma_{\text{min}}}{\sigma_{\text{max}}}
$$
1.2 Experimental observations of the studied materials

Figure 1.2.1: Terminology of the loading in a standard stress controlled fatigue test

The results of fatigue tests are usually presented in the so-called S-N curve: the stress level ($\sigma_{\text{amp}}$ or $\sigma_{\text{max}}$) as a function of the number of cycles to failure ($N_f$), in a logarithmic scale (cf. figure 1.2.6 for example).

1.2.1 Short fiber reinforced thermoplastic polymers

Several experimental studies have demonstrated the importance of effects related to the complex microstructure of SFRTPs and influencing factors due to mechanical and environmental working conditions, mainly: temperature and humidity variation. These effects will be detailed in the following paragraphs, starting from the effects of microstructure. Due to the material composition: polymer matrix and misaligned short fibers, the behavior is very complex under regular loading and more complex at loading causing failure such as fatigue. The evaluation of those effects is accomplished using standard fatigue tests, under uniaxial and multiaxial loading. Special geometries of specimens are used in the case of torsion and compression fatigue test such as tubular specimens, in order to avoid structural instabilities like buckling.

1.2.1.1 Influence of the microstructure composition

The most common TPs used as matrix materials are Polyamide (PA), polypropylene (PP) and thermoplastic polyesters such as polybutylene terephthalate (PBT) and polyethylene terephthalate (PET). The matrix behavior plays a key role in the behavior of SFRTPs. Standard materials used for fiber reinforcement are glass, carbon, and boron. Glass fibers are the most used (95%) due to their low cost, high strength, chemical resistance and insulating properties (Biron, 2012; Mortazavian and Fatemi, 2014). The microstructure influences on the material behavior were investigated mainly based on the effects of the fibers concentration, their orientations and the interface between them and the matrix. In the following paragraphs, some works realized to study these influences are presented.
1.2 Experimental observations of the studied materials

Effect of fiber fraction or content  The fiber volume fraction effect was evaluated under both monotonic loadings and fatigue. Under static loading, the increase of the fiber concentration increases the stiffness and strength level, as observed for example by Mouhmid et al. (2006) on SFRP66 (see figure 1.2.2). Under fatigue loading, the lifetime tends to increase, with the increase of the fiber volume fraction according to several authors (eg. Zago and Springer, 2001b; Launay et al., 2011a).

![Figure 1.2.2: Stress–strain curves for SGRPA.66 with different glass fiber concentrations at 20°C and strain equal to 5.610^-3s^-1](From Mouhmid et al., 2006).

Effects of fiber orientation distribution (FOD) and fiber length distribution (FLD)  The majority of SFRTPs parts are obtained by an injection molding process, which gives complex fiber orientation distributions (FOD) related to the complex flow field (Mortazavian and Fatemi, 2014). As a result, not only the FOD will change from one small volume to another within an injected part but a layered structure is usually observed in the thickness, defined by skin, shell, and core layers (Arif et al., 2014a; De Monte et al., 2010a; Horst and Spoormaker, 1996), (cf. figure 1.2.3 for an example of the microstructure of PA66/GF30 observed by Arif et al. (2014b)). In the shell layers the fibres are mainly oriented parallel to main flow direction (MFD) (De Monte et al., 2010c). The degree of fiber alignment has an important and a similar effect on both tensile and fatigue properties (Horst and Spoormaker, 1996, 1997).
1.2 Experimental observations of the studied materials

Figure 1.2.3: Skin–shell–transition–core microstructure formation of PA66/GF30 observed by µCT technique (Arif et al., 2014b), where MFD is the mold flow direction.

Generally the specimens are cut from an injected plate at different angles w.r.t. the MFD, in order to measure the influence of the anisotropy on the material behavior (cf. illustration in figure 1.2.4). The figure 1.2.5 from De Monte et al. (2010c) shows that the longitudinal and transverse tensile properties w.r.t. MFD, are different. The fibers enable to carry the maximum of load, when it is applied in their principal direction, thus the longitudinal direction allows to reach higher level of stress. This observation can be seen also in the case of fatigue loading (cf. figure 1.2.6 on PA66/GF30), the level of stress and the lifetime are higher, when the loading is applied in the longitudinal direction, as observed also by Zhou and Mallick (2006) in the case of PA66/GF33 under axial fatigue. Indeed, they noticed that the material tensile strength and fatigue strength are higher in MFD than normal to it, similar observations were made by other authors (eg. Bernasconi et al., 2007; Klimkeit et al., 2011a).
1.2 Experimental observations of the studied materials

Figure 1.2.4: Different specimens cut-out at different angle w.r.t. MFD

Figure 1.2.5: Effects of orientation and temperature on stress–strain curves for 1 mm thick specimens of PA66-GF35, at room temperature (RT) and 130 °C (From De Monte et al., 2010c).
1.2 Experimental observations of the studied materials

Figure 1.2.6: S–N curves for different directions w.r.t. MFD for PA66-GF30. Maximum stresses are normalized.

The effect of fiber length distribution (FLD) was much less investigated experimentally. Typical fiber lengths are in the range 25–550 µm. According to Launay et al. (2013b) the slope of S-N curves seems to be independent of FLD.

**Interface between fiber and matrix** The interface between fiber and matrix plays a very important role in material behavior. The interface is responsible of the stress transfer between matrix and fibers. The important difference in terms of mechanical properties between the two materials can justify the material behavior sensitivity to the fiber aspect ratio change, i.e. change of the contact surface. Chemical coupling agents, such as silane, are generally used in order to improve the bonding between matrix and fibers (Mortazavian and Fatemi, 2014). Several works tried to investigate the effect of the fiber matrix interface on the material behavior under fatigue loading, such as Takahara et al. (1994) who investigated the effect of strengthening the interfacial adhesion between glass fiber and PBT matrix, and concluded that it improves the fatigue strength. Similar conclusions were already given by Mandell et al. (1983) for several short fiber-reinforced thermoplastics, and they checked that a well-bonded interface for reinforced nylon 6.6 gives matrix-controlled fatigue sensitivity.

1.2.1.2 Effects of a part’s working conditions

A part undergoes a large number of effects during its use, mainly mechanical and environmental: temperature and humidity variation. Among the mechanical effects under cyclic loading, the so-called **mean-stress effect** is a well

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1 Abstract

1.2 Experimental observations of the studied materials

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The fiber aspect ratio is the ratio of length to diameter of a fiber
known effect in fatigue testing for almost all materials. It happens if the loading ratio ($R$) varies. The mean stress effect proves the non-linearity of the material failure behavior (cf. figure 1.2.7 showing an example of S-N curves for PA66GF33 under a tensile fatigue loading with different value of $R$). For positive mean stress, the effect of creep was also observed by several authors such as (Zhou and Mallick, 2006; Mallick and Zhou, 2004), at both low and high frequencies on PA66GF33 under a constant amplitude and various maximum stress (cf. figure 1.2.8).

![Figure 1.2.7: Mean strain as a function of time at different maximum fatigue stress levels for PA66/GF33 (Mallick and Zhou, 2004)](image)

The resulting response is an interaction between creep and fatigue damage as mentioned in several works such as Launay et al. (2011a) and Horst and Spoormaker (1996). The creep contribution to material behavior could be explained by the viscous nature of the material, which is also responsible for various other effects such as temperature and loading rate sensitivities, as it will be detailed hereafter.
1.2 Experimental observations of the studied materials

Figure 1.2.8: Mean strain as a function of time at different maximum fatigue stress levels for PA66/GF33 (Mallick and Zhou, 2004)

**Loading rate, frequency and self heating effects** Under tensile loading, the level of stress for a fixed value of deformation increases when the stress or strain rate increases, whether the water content is important or not, as shown by (Launay et al., 2011a) for PA66/GF30 (cf. figure 1.2.9). Under axial fatigue loading, Zhou and Mallick (2006) showed that the fatigue of PA66/GF33 is sensitive to frequency especially when it is higher than 2Hz, and the fatigue life decreased with increasing frequency, due mainly to self heating (cf. figure 1.2.10).

The TPs matrix is known to have a low thermal conductivity, so the heat generated during the loading (stress or strain controlled) is not transferred totally to the external environment of a part and causes further irreversible deformations. Self heating is important especially under high frequencies and loading rates. It is generally noticed experimentally that if the size increase of hysteresis loops is important, then self heating or commonly called *hysteresis heating* is important and the fatigue is qualified as *thermal*, in the other case it is called *mechanical*. The fiber-matrix interface plays an important role on hysteresis heating (e.g. Lang and Manson, 1987; Subramanian and Senthilvelan, 2009) who studied the effect of fiber length on this heating.
1.2 Experimental observations of the studied materials

Figure 1.2.9: Strain-stress curves under monotonic tensile tests for SGFRPA66 on Dry-as-molded (DAM) [continuous lines] and RH50 [dashed lines] materials, at various stress rates. (Launay et al., 2011a)

Figure 1.2.10: Effect of cyclic frequency on the fatigue life of PA66 reinforced with 30% of volume fraction of glass fibres ($R=0.1$) (Zhou and Mallick, 2006).
1.2 Experimental observations of the studied materials

**Temperature and relative humidity** As already mentioned, the parts made with SFRTPs are submitted during their lifetime to changes in temperature and relative humidity. Several authors tried to investigate the effect of the former environmental effects, such as De Monte et al. (2010b); Zhou and Mallick (2006). The effect of temperature on PA66/GF35 was investigated under quasi-static (De Monte et al., 2010c) and cyclic loadings (De Monte et al., 2010b). The increase of temperature usually decreases both the tensile (cf. figure 1.2.5) and fatigue strengths.

The water content has a similar important influence on SFRTPs. Usually, this influence is quantified by using specimens that are dry-as-molded (DAM) or saturated. Under monotonic loading, Mouhmid et al. (2006) mentioned that the tensile strength in glass fiber reinforced PA66 is 50% higher in the dry state than in the saturated one, this is confirmed by (Launay et al., 2011a) for SGFRPA66 (cf. figure 1.2.9). Under fatigue loading, this influence is also important as mentioned by Horst and Spoormaker (1996) on the failure mode of the PA6 matrix. More recent works tried to study this effect such as Barbouchi et al. (2007); Launay et al. (2013c); Arif et al. (2014a). According to Launay et al. (2013c) the effects of temperature and relative humidity on the cyclic behavior and fatigue life are similar and coupled, probably because higher water content in the matrix results in lower glass transition temperature.

1.2.1.3 Failure and damage mechanisms

The failure and damage mechanisms of SFRTPs were investigated under monotonic and fatigue loadings by several authors. Having an accurate idea about the mechanisms and establishing a failure scenario are crucial steps, in order to obtain reliable modeling approaches. Due to the complexity of the material microstructure, macroscopic observations (e.g. Bellenger et al., 2006) at the scale of the work-part are not sufficient to obtain an accurate knowledge about the damage mechanisms, especially when the failure occurs suddenly with no visible degradation of the material physical characteristics at macroscale. Hence investigations at the microscopic scale that of microstructure seem to be more suitable for characterizing the phenomena. Various experimental tools were employed such as scanning electron microscopy (SEM)(e.g. Mouhmid et al., 2006; Arif et al., 2014b) and fractographic studies (e.g. Horst and Spoormaker, 1996, 1997).

**Under monotonic loading** In order to visualize the damage process under monotonic loadings, several authors such as Sato et al. (1991) and Mouhmid et al. (2006) analyzed the fracture surface of specimens using SEM. They reported that the damage mechanisms in PA/GF are characterized by matrix plasticization and micro-cracks, fiber pull-out and fracture. Their microscopic observations showed that damage is localized in the matrix near the fiber interface as depicted in picture 1.2.11, where the stress concentration is important as shown by FE computation that we performed (see figure 1.2.12). Sato et al. (1991) proposed a damage mechanism described by a crack which starts from fibers ends and propagates along the fiber–matrix interface (cf. figure 1.2.13).
1.2 Experimental observations of the studied materials

Figure 1.2.11: A cluster of microcracks occurring in the matrix around the fiber tip, which was obtained under about 50% of failure load. (Sato et al., 1991)

Figure 1.2.12: A graphical presentation of von Mises stress distribution obtained with a FE computation of a 3D cell composed of a PA66 matrix (assumed to have an elastoplastic behavior) reinforced with short glass fibers, under monotonic tensile loading applied in the fiber direction.
1.2 Experimental observations of the studied materials

Figure 1.2.13: Failure mechanism in monotonic tension along main fibers’ direction proposed by Sato et al. (1991). Damage is initiated at the ends of fibers, cracks propagate in fiber matrix interface, then a plastically deformed zone develops. In this zone a ductile crack will propagate rapidly to give the final failure of the material. Microscopic observations show that the fibers are not broken even at the final stage of fracture.

Under fatigue loading Several authors investigated the damage mechanisms under fatigue loadings, (e.g. Horst and Spoormaker, 1996, 1997; Noda et al., 2001; Casado et al., 2006; Arif et al., 2014a). Horst and Spoormaker studied also the fracture surface and proposed a damage mechanism similar to the one of Sato et al. (1991). They noticed the important role of stress concentration at fiber tips. Two damage mechanisms were proposed depending on whether the specimen is dry as-molded (DAM) or conditioned. According to their observations, the matrix has a brittle behavior when it is DAM, and a ductile behavior in the other case. Horst and Spoormaker (1996, 1997) proposed a mechanism that consists of the following steps: damage begins with void formation, mainly at fibers ends; these voids coalesce into small cracks, which will propagate into the material, and give the final failure (see figure 1.2.14 for a schematic presentation of the proposed damage mechanism). Others authors later confirmed the proposed mechanisms and proposed similar ones. However two stages are almost always respected, which are crack initiation and its propagation. The initiation stage remains an open research field (Launay et al., 2013b).
1.2 Experimental observations of the studied materials

![Idealized failure mechanism in fatigue proposed by (Horst and Spoormaker, 1996, 1997), based on fatigue tests in the main flow direction (MFD). Damage is initiated at the location of highest stress intensity, the fibre ends, 1. Voids grow from this damage, along the fibres, 2. In a small percentage of cases, voids develop in the middle of a fibre, or at a fractured fibre. These voids grow, 3, and coalesce, 4, but no complete crack will develop. Both “crack” walls remain connected by bridges, which occur mainly at the specimen surface.](image)

Recently, Klimkeit et al. (2011a) investigated the fatigue damage mechanisms of a short glass-reinforced PolyButylene Terephthalate and Polyethylene Terephthalate with the fiber volume fraction of 30% (PBT+PET GF30) and different fiber orientations at loading ratio $R=0.1$, using multiple techniques: replica technique, Infrared imaging and scanning electron microscopy. They confirmed the same mechanisms, however they added that damage observed along the fibers sides is related to spatial distribution of fibers rather than stress distribution around one single fiber, and they confirmed that the duration of the propagation phase of the macrocrack is too small compared to the lifetime of the material. More recently, Arif et al. (2014b,a) investigated the effect of relative humidity on the SGFRPA66 damage mechanism. Their investigations confirmed the observations of (Horst and Spoormaker, 1996, 1997) and their proposed damage mechanism.

In conclusion, the damage mechanisms are very complex, and they depend on the TP’s matrix behavior, the interface treatment between the fibers and the matrix. However the phenomena can be summarized in an idealized way in order to have a failure scenario which is realistic enough to justify the proposed modeling approaches. It is clear that the matrix behavior plays an important role, and that the damage is initiated at the fiber tips mainly. The interface between fiber and matrix is also important, while fibers failure seems to be
1.2 Experimental observations of the studied materials

much less likely to happen under fatigue loading since the stress state seems to be generally low enough compared to the failure limit state of the fibers. The contribution of the matrix behavior seems to be a key element in the behavior and failure of SFRTPs. This conclusion is shared by several works such as Mourglia-Seignobos (2009). In the following paragraph a brief literature review about the behavior of unreinforced TPs is given.

1.2.2 Unreinforced thermoplastic polymers

Thermoplastic polymers behavior depends on many factors, namely strain rate (cf. figure 1.2.15 for PA66), temperature, pressure, water content (Mouhmid et al., 2006), etc.

![Stress-strain curves of unreinforced PA66 for different strain rates](image)

Figure 1.2.15: Stress–strain curves of unreinforced PA66 for different strain rates: (Mouhmid et al., 2006)

The failure of thermoplastic polymers was investigated experimentally under various loading conditions and at different scales. Macroscopic investigations showed a decrease of the material’s stiffness and strength during loading. Examples include the damage and failure observations of Boisot et al. (2011) on notched Polyamide 11 specimens and those of Uchida and Tada (2011) on neck propagation under tensile loading, combined tension-torsion fatigue tests on polypropylene (Berrehili et al., 2010a,b), fatigue cyclic loading of HDPE (Drozdov, 2011), creep of HDPE (Krishnaswamy, 2005), creep rupture and chemical aging (Crissman and McKenna, 1987, 1990) and of PA6 (Sai et al., 2011).

Some microscopic investigations of the TPs failure (e.g. Kausch, 1978; Friedrich, 1983) have related damage to the creation of micro-voids, their enlargement and coalescence. Other microstructure investigations related damage to plasticity within the materials (e.g. Détrez, 2008; Detrez et al., 2011). According to Narisawa and Ishikawa (1990), failure results from two mechanisms: crazing and plastic yielding.
1.2 Experimental observations of the studied materials

Under fatigue loading, two different behaviors are usually distinguished: thermally dominated behavior and mechanically dominated behavior, as shown by the S-N curve of Polyactal (Lesser, 1995) (cf. figure 1.2.16). The thermally dominated regime may be obtained in the case of high frequency or high level of applied strain or stress, however the thermally dominated regime is obtained in the case of low frequencies and low level of stresses or strains. Between the two regimes a transition plateau is usually present. These two tendencies are described in more detail in (Sauer and Richardson, 1980; Lesser, 2002) for example. A difference in terms of hysteresis loops is usually considered as an indicator of the two regimes, as shown in figure 1.2.16, the larger the hysteresis loops, the higher the energy dissipation within the material leading to the so-called thermal softening.

Figure 1.2.16: Plots of hysteresis loops for Polyactal fatigued in the low cycle (thermally dominated) and high cycle (mechanically dominated) regions. (Lesser, 1995)

As shown by the experimental results of (Berrehili, 2010; Berrehili et al., 2010b,a) (see figure 1.2.17), for the same test with identical testing conditions, the material may fail or not, although the level of strains is comparable. This may be explained by the initiation of the macroscopic instability at a lower scale than the parts scale.
1.2 Experimental observations of the studied materials

Figure 1.2.17: Comparison of the variation of the maximum equivalent strain in HDPE, vs. the number of cycles, at maximum von Mises equivalent stress equal to 24.4 MPa and loading ratios R=0 and R=-1: (a) for the short tests, (b) for the long tests (From Berrehili, 2010)

In order to predict fatigue life of the polymers, several failure scenarios and experimental interpretations were employed to motivate the chosen approaches. The most famous one is that the material instabilities start at a microscale and caused by crack initiated at preexisting defects or inhomogeneities within the material or low density domains formed at nanometric scale as proposed by Mourglia-Seignobos et al. (2014) for fatigue failure of PA66.

The fatigue of polymers seems to occur mainly in two stages, a first stage of progressive degradation of material mechanical properties until the initiation of a crack, and a second stage when the initiated crack propagates up to the final fracture of the work-part (Kallrath et al., 1999). See an example the failure
1.3 Thesis scope and objectives

According to Lesser (2002) the crack initiation stage takes about 95% of the fatigue lifetime in the case of polymers. Sauer and Chen (1983) showed similar conclusions for high-impact polystyrene (HIPS) and polystyrene (PS). Janssen et al. (2008a) showed that based on fatigue tests on samples of PC, polypropylene (PP), and PMMA, the initiation stage almost covers the entire fatigue life (>99%).

![Fracture surface in Polyactal resin specimen subjected to tensile fatigue](image)

Figure 1.2.18: Fracture surface in Polyactal resin specimen subjected to tensile fatigue (Lesser, 2002)

1.3 Thesis scope and objectives

The main objectives of this thesis are to numerically predict the damage and failure of both unreinforced thermoplastic polymers (TPs) and misaligned short fiber reinforced thermoplastic polymers (SFRTPs), mainly under mechanical fatigue loading with large number of cycles: high cycle fatigue (HCF). The modeling approaches should take into account multiaxial stresses and the microstructure of the studied materials. In order to predict the effective response of the studied heterogeneous materials from their microstructure, multiscale approaches are employed, based on mean-field homogenization methods.

The short review about the experimental observations on the SFRTPs behavior, presented in the previous section, evidenced a complex behavior that depends on the material microstructure namely the fibers content, their orien-
1.3 Thesis scope and objectives

tation and length distribution and also the TPs matrix and its interface with the fibers. In order to obtain a realistic modeling approach for the SFRTPs fatigue an overview about existing failure scenarios based on experimental studies were summarized. The common conclusion between those proposed scenarios is relating the failure of the material to the initiation of a crack and its propagation until the final failure of the material. For several types of SFRTPs the crack initiation seems to govern the lifetime of the material. On the other hand the initiation stage is defined by a progressive deterioration of the material that is most likely to happen in the TPs matrix and the fiber-matrix interface at limited zones.

About the failure of the unreinforced thermoplastics under monotonic loading, the failure mechanisms are very complex and they depend on the applied loading and working conditions of the studied part. We chose to link the damage and failure under monotonic loadings to irreversible deformations within the material as proposed by some authors, and as already mentioned in the experimental observations section.

Under fatigue loading, the final fatigue failure may also be defined by a crack initiation stage and a propagation stage. According to several authors, as already mentioned, the initiation stages may define for several TPs the majority of the lifetime, similar to SFRTPs. The initiation of the cracks seems to start also at limited zones that may correspond to preexisting defects or inhomogeneities within the material.

In this work, several modeling approaches are proposed based on the previous experimental observations. In order to model the progressive failure of unreinforced TPs under monotonic loading, which is defined by a largely diffused damage within the material, assumed to be related to irreversible deformations, a new constitutive model coupling linear viscoelasticity, viscoplasticity and damage (VEVPD) is proposed. This model was used to simulate the behavior of various thermoplastic polymers under monotonic loadings.

On the other hand, based on the idea that the fatigue failure of SFRTPs and TPs may be related to progressive damage within limited zones of the studied material, the so-called weak spots concept is employed to model those zones. They are assumed to obey to the VEVPD behavior model. Two modeling approaches are proposed for both unreinforced TPs and SFRTPs. For each approach, the composition of the volume element where the fatigue failure may happen is proposed.

For the fatigue behavior of TPs, the volume element is defined by an undamaged matrix assumed to obey a VE behavior and containing weak spots having VEVPD behavior (cf. figure 1.3.1).
1.3 Thesis scope and objectives

Figure 1.3.1: Multiscale damage model for HCF of homogeneous thermoplastic polymer materials

A similar modeling approach is proposed for SFRTPs (cf. figure 1.3.2), where the considered volume element is composed of VE matrix, weak spots and misaligned short fibers. The injection molding manufacturing process is taken into account through the concentration and orientation of the misaligned fibers. Mean-field homogenization techniques are used in order to evaluate the stress and strain states within phases for each proposed volume used in the modeling approaches for fatigue.

Figure 1.3.2: Multiscale damage model for HCF fatigue of short fiber reinforced thermoplastic polymer materials

A new mean field homogenization model is proposed for VEVPD composites, where both the matrix and the inclusions are assumed to be VEVPD based on a incrementally affine linearization method. The MFH method is used to measure the interaction between the different phases, for each volume element.
1.4 Thesis synopsis

This thesis is organized as follows. For each chapter a description of the state of the art in modeling approaches is given, followed by a proposed modeling approach for the chapter problem.

In chapter 2, the new constitutive model for materials with coupled linear viscoelasticity, viscoplasticity and damage (VEVPD) is proposed in order to model the behavior of TPs when the damage is largely diffused within the material. The constitutive equations and the numerical algorithms are detailed. The model is employed to predict the behavior of several TPs under monotonic loadings.

An overview about the existing mean-field methods for linear and nonlinear composites is presented in chapter 3. The chapter also contains a mean-field homogenization model proposed for VEVPD composites, where both the matrix and the inclusions are assumed to be VEVPD.

The developed mean-field model is used in chapter 4 in order to model the interaction between a viscoelastic TPs matrix and VEVPD weak-spots. An overview about the existing modeling approaches of TPs fatigue is given, in order to classify the proposed model in the existing literature and highlight its advantages. The model is evaluated and compared to experimental results. Possible enhancements are also presented in that chapter.

Chapter 5 focuses on the fatigue of SFRTPs. An overview about the existing modeling approaches for this problem is presented. The proposed model is detailed and evaluated against experimental results on fatigue of SGFRPA66. Conclusions and possible enhancements of the modeling approaches are presented in chapter 6.

1.5 Supporting publications


- Krairi, A., Doghri, I., A two-scale model for the high cycle fatigue of neat thermoplastic polymers (In preparation).

- Krairi, A., Doghri, I., A multiscale model for the high cycle fatigue of SFRTPs (In preparation).
Chapter 2

A thermodynamically-based constitutive model for thermoplastic polymers coupling viscoelasticity, viscoplasticity and ductile damage

This chapter\textsuperscript{1} presents a thermodynamically-based constitutive model for isotropic homogeneous thermoplastic polymers under non-monotonic and arbitrary multiaxial loadings. The model couples viscoelasticity, viscoplasticity and ductile damage. The chapter is organized as follows: section 2.1 gives a description of the state of the art, then section 2.2 presents a detailed development of the constitutive model based on a thermodynamics framework. In section 2.3, numerical predictions are validated against experimental tests on different polymers under various loadings. Finally, a discussion and possible enhancements of the model are presented in section 2.4.

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\end{itemize}

\textsuperscript{1}Some developments of this chapter led to the publication "A thermodynamically-based constitutive model for thermoplastic polymers coupling viscoelasticity, viscoplasticity and ductile damage" in International Journal of Plasticity Krairi and Doghri (2014)
2.1 State-of-the-art description

Mainly two approaches to model progressive damage have been pursued. The first approach is motivated by the idea of relating damage to the growth and coalescence of voids and is based on micro-mechanics models such as Gurson's model (Gurson, 1975, 1977). The second one is continuum damage mechanics (CDM) such as Lemaitre's model, motivated by linking damage-modeled as elastic stiffness decrease-and plastic strain evolutions within the material. The Gurson model is well known in modeling ductile damage of metallic materials through several phenomenological modifications to its initial version (Tvergaard, 1982, 1981; Tvergaard and Needleman, 1984; Tvergaard, 1990; Tvergaard and Hutchinson, 1992; Gologanu et al., 1993; Pardoen et al., 1998). It was also used and modified for several other types of materials such as rubber-toughened polymers (Lazzeri and Bucknall, 1995; Jeong and Pan, 1995; Steenbrink et al., 1997; Pijnenburg and Van der Giessen, 2001; Zairi et al., 2005, 2008), semi-crystalline polymers (Laiarinandrasana et al., 2009; Boisot et al., 2013) and other materials. The CDM approach is based on the concept of damage variable and effective stress introduced by Kachanov (1958) and Rabotnov (1963). This concept reflects various types of damage at the microscopic scale through their effect phenomenologically at the macroscopic scale. CDM was formulated in the framework of thermodynamics of irreversible processes by Lemaitre and Chaboche (1978). It was originally developed for metallic materials, assumed to be elastoplastic (Lemaitre and Chaboche, 1978; Lemaitre, 1985b,a; Wanjia et al., 1992; Lemaitre and Doghri, 1994; Chaboche, 1997; Abu Al-Rub and Voyiadjis, 2003; Voyiadjis and Dorgan, 2007; Haddag et al., 2009). CDM was used for other types of materials as well, such as rubber-toughened polymers Tang and Lee (1995); Miehe and Keck (2000), mineral filled semi-crystalline polymers assumed to be elastoviscoplastic Balieu et al. (2013), asphalt concrete assumed to be a viscoelastic-viscoplastic material (Uzan, 2005; Zhu and Sun, 2012), rubber-like materials assumed to be visco-hyperelastic (Ayoub et al., 2012, 2011b, 2013, 2011a) and other materials. Recently several generalizations of standard CDM have been proposed such as continuum damage healing mechanics (CDHM) for glassy polymers based on self healing system (Voyiadjis and Dorgan, 2007; Darabi et al., 2011; Voyiadjis et al., 2011; Abu Al-Rub and Durabi, 2012; Voyiadjis et al., 2012).

In order to take into account softening and physical aging of thermoplastics, another type of models is proposed in the literature developed based on the original works of Haward and Thackray (1968); Boyce et al. (1988); Hasan and Boyce (1995); Govaert et al. (2000). They may be classified in the same class as CDM approaches since they couple those effects to the plastic deformation. A finite strain elasto-viscoplastic formulation is employed. The softening and the physical aging are taking into account using a viscoplastic function that was modified by several authors such as (Govaert et al., 2000; Klompen et al., 2005). The version proposed by Klompen et al. (2005) was used by Janssen et al. (2008a) in order to predict the behavior of materials under fatigue loadings. Hereafter, some constitutive equations of the model are given. The total stress is split into a driving stress $\sigma_s$ corresponding to the stress contribution of
2.1 State-of-the-art description

the intermolecular interactions and another part $\sigma_r$ representing the strain hardening contribution (cf. figure 2.1.1 for illustration).

$$\sigma = \sigma_r + \sigma_s$$  \hspace{1cm} (2.1.1)

The stress $\sigma_r$ is modeled with a single neo-Hookean spring. The stress $\sigma_s$ gives the non-linearity of the model and is function of a viscosity function defined in Klompen et al. (2005) as follows:

$$\eta(T, \bar{\tau}, p, S) = \eta_{0,r} (T) \frac{\bar{\tau}/\tau_0}{\sinh (\bar{\tau}/\tau_0)} \exp \left( \frac{\mu p}{\tau_0} \right) \exp (S(t, \bar{\eta}_p))$$  \hspace{1cm} (2.1.2)

where $\eta_{0,r} (T)$ is the zero viscosity for the completely rejuvenated state and $\bar{\tau}$ is the equivalent stress computed from the stress $\sigma_s$. The stress dependence of the viscosity is governed by the parameter $\tau_0$, the pressure dependence by the parameter $\mu$, while $p$ is the hydrostatic pressure. The material state $S$ is determined by two processes: physical aging, measured as an increase in yield stress, and mechanical rejuvenation during loading, measured as true strain softening. The models are able to take into account the pressure and temperature dependencies under several cases of loading mainly monotonic, but they can’t model the material behavior under cyclic loading, namely the hysteresis loops (cf figure 2.1.2).

Figure 2.1.1: Schematic representation of the elasto-viscoplastic model. Where $G$ is the shear modulus and $G_r$ is the strain hardening modulus (Janssen et al., 2008a)
2.2 Proposed model

This work is devoted to modeling the nonlinear deformation and progressive damage under small strain hypothesis and isothermal conditions for thermo-plastic polymers using CDM approach. The proposed model includes two important contributions. The first one is that it couples VE, VP, nonlinear isotropic and kinematic hardenings and damage. The second contribution is that the model is written rigorously within the formalism of the thermodynamics of irreversible processes, under general multi-axial, non-monotonic and non-proportional loadings. The thermodynamics framework is inspired by the works of Christensen (1982) on VE and Lemaitre (1985b); Chaboche (1997) on VP and damage. The total strain is decomposed into VE and VP parts. The undamaged Cauchy stress depends on the history of VE strains through Boltzmann’s integral. VE bulk and relaxation moduli follow general Prony series. The VP response combines isotropic and nonlinear kinematic hardenings. In this work, damage is called “ductile” because by construction it only evolves when there is a change in the VP strains. Closed-form and rather simple expressions of the strain energy density release rate and of the different dissipation terms are found. Time and strain rate dependencies, the Baushinger effect and ductile damage are modeled.

The thermodynamics of irreversible processes is developed in this section for the proposed model. It is assumed, as in (Nikolov and Doghri, 2000; Voyiadjis et al., 2011; Miled et al., 2011), that for a polymer the total strain is decomposed into two parts: a viscoelastic (VE) strain $\varepsilon^{ve}$ and a viscoplastic (VP) one $\varepsilon^{vp}$:

$$\varepsilon = \varepsilon^{ve} + \varepsilon^{vp}$$  \hspace{1cm} (2.2.1)
2.2 Proposed model

For semi-crystalline polymers, \( \varepsilon^{ve} \) could be attributed to the amorphous phase and \( \varepsilon^{vp} \) to the crystalline one. Also, in a monotonic tension test in the 1-direction, once a total strain \( \varepsilon_{11} \) has been reached, if we unload to zero stress (\( \sigma_{11} = 0 \)) and wait for a long time, then the residual strain is the VP one (\( \varepsilon_{11}^{vp} \)) while the VE strain is \( \varepsilon_{11}^{ve} = \varepsilon_{11} - \varepsilon_{11}^{vp} \).

The Helmholtz free energy function \( \psi \) is decomposed into a viscoelastic part coupled with damage and denoted by strain energy function \( \psi^{ve} \) and a hardening function \( \psi^{h} \).

\[
\psi = \psi^{ve} + \psi^{h}
\]

(2.2.2)

The expression of \( \psi^{ve} \) is defined as:

\[
\rho \psi^{ve}(t) = \frac{1}{2} (1 - D(t)) \int_{-\infty}^{t} \int_{-\infty}^{t} \frac{\partial \varepsilon^{ve}(\tau)}{\partial \tau} : \mathbb{C}^{ve} (2t - \tau - \eta) \frac{\partial \varepsilon^{ve}(\eta)}{\partial \eta} d\tau d\eta
\]

(2.2.3)

where \( \rho \) denotes the material density and is assumed to be constant, and \( \mathbb{C}^{ve} \) is the relaxation tensor having the minor symmetries: \( \mathbb{C}^{ve}_{ijkl} = \mathbb{C}^{ve}_{ikjl} = \mathbb{C}^{ve}_{ijlk} \) and the major ones \( \mathbb{C}^{ve}_{ijkl} = \mathbb{C}^{ve}_{klij} \). The expression of \( \psi^{ve} \) is defined similarly to Christensen (1982), with two important differences. The first one is that the history of VE strains (\( \varepsilon^{ve} \)) is involved instead of the total ones (\( \varepsilon \)). The second difference is the coupling with damage variable (\( D \)). Let us remark that in the VEPD model of Zhu and Sun (2012) the damage and the VE contributions are uncoupled, and the expression of \( \psi^{ve} \) is not given. The hardening part of the energy is defined as in (Doghri, 1993) as:

\[
\rho \psi^{h}(t) = \frac{a}{2} \alpha(t) : \alpha(t) + \int_{0}^{\eta(t)} R(\xi) d\xi
\]

(2.2.4)

In this work, \( \{\varepsilon^{vp}, V = \{r, \alpha, D\}\} \) are internal variables, to which thermodynamic forces are associated (\( \sigma, A = \{R, X, -Y\}\)). The scalar variable \( r \) models isotropic hardening and the strain-like tensor \( \alpha \) models kinematic hardening. The scalar variable \( R \) measures the radius of the yield surface in the space of the deviatoric stresses while the variable \( X \) measures the translation of the center of that surface in the same space. The internal scalar variable \( D \) models the damage, which is assumed to be isotropic and varies between 0 (for sound material) and 1 (complete failure). The thermodynamic force associated to \( D \) is denoted by \( Y \).

The Clausius-Duhem inequality requires the dissipation \( \phi \) to be non-negative and in the isothermal case it reads:

\[
\phi = \sigma : \frac{d\varepsilon}{dt} - \rho \frac{d\psi}{dt} \geq 0
\]

(2.2.5)

2.2.1 Thermodynamic derivation

In appendix A, using Leibniz rule to carry out the time derivation of equation (2.2.3), the following expression of the Cauchy stress is found:
2.2 Proposed model

\[ \sigma(t) = (1 - D(t)) \int_{-\infty}^{t} C^{ve}(t - \eta) : \frac{\partial \epsilon^{ve}(\eta)}{\partial \eta} d\eta \quad (2.2.6) \]

The Cauchy stress \( \sigma(t) \) is thus related to the damage variable \( D(t) \) and to the whole history of VE strains \( \epsilon^{ve}(\eta) \) via Boltzmann’s hereditary integral. The relation between the Cauchy stress \( \sigma(t) \) and the so-called effective stress \( \tilde{\sigma}(t) \) is:

\[ \tilde{\sigma}(t) = \frac{\sigma(t)}{1 - D(t)} \quad (2.2.7) \]

In uniaxial tension, if \( F(t) \) and \( A(t) \) designate the current load and total cross section area, respectively, then:

\[ \sigma_{11}(t) = \frac{F(t)}{A(t)}; \quad \tilde{\sigma}_{11}(t) = \frac{F(t)}{\tilde{A}(t)}; \quad \tilde{A}(t) = (1 - D(t))A(t) \quad (2.2.8) \]

where \( \tilde{A}(t) \) is the undamaged part of \( A(t) \). Equation (2.2.7) is thus obtained. For a given total strain \( \epsilon_{11}(t) \), in monotonic uniaxial tension, figure 2.2.1 illustrates the difference between \( \sigma_{11}(t) \) and \( \tilde{\sigma}_{11}(t) \).

\[ \text{Figure 2.2.1: Illustration of effective stress concept in monotonic uniaxial tension test} \]

The expressions of the other thermodynamic forces are derived according to:

\[ A = \rho \frac{\partial \psi}{\partial V} \quad (2.2.9) \]

Isotropic and kinematic hardenings are then expressed as:

\[ R = R(r), \quad X = a\alpha, \quad (2.2.10) \]

An example of isotropic hardening is the power law defined as:
2.2 Proposed model

\[ R(t) = kr^n \tag{2.2.11} \]

where \( k [Pa] \) and \( n \) are the hardening modulus and exponent, respectively. The damage thermodynamic force \( Y \) (or the strain energy density release rate, as known in CDM) is associated with the damage variable \( D \) and defined from equations (2.2.9) and (2.2.3) as (see appendix A):

\[ Y(t) = \frac{1}{2} \int_{-\infty}^{t} \int_{-\infty}^{t} \frac{\partial \xi^{ve}(\tau)}{\partial \tau} : C^{ve}(2t - \tau - \eta) : \frac{\partial \xi^{ve}(\eta)}{\partial \eta} \, d\tau d\eta \tag{2.2.12} \]

As demonstrated in appendix A, the intrinsic dissipation in the isothermal case is given by:

\[ \phi = \sigma : \dot{e}^{vp} + Y \dot{D} + (1 - D)\phi^{ve} - X : \dot{\alpha} - R(t) \dot{t} \geq 0 \tag{2.2.13} \]

where

\[ \phi^{ve} (t) = - \int_{-\infty}^{t} \int_{-\infty}^{t} \frac{\partial \xi^{ve}(\tau)}{\partial \tau} : \frac{\partial C^{ve}(2t - \tau - \eta)}{\partial t} : \frac{\partial \xi^{ve}(\eta)}{\partial \eta} \, d\tau d\eta \tag{2.2.14} \]

\( \phi^{ve} \) is the viscoelastic part of the intrinsic dissipation. For elastic (visco)plastic behavior, \( \phi^{ve} (t) = 0 \) because the relaxation tensor \( C^{ve} \) is constant over time and equal to Hooke’s operator. Note that in the VEVPD model proposed by Zhu and Sun (2012) for asphalt mixtures, the VE dissipation \( \phi^{ve} \) is ignored completely in equation (2.2.13).

For an isotropic material \( C^{ve} \) could be written as follows:

\[ C^{ve}(t) = 2G(t)I^{dev} + 3K(t)I^{vol} \tag{2.2.15} \]

where \( G(t) \) and \( K(t) \) are shear and bulk relaxation functions, resp., which can be expressed using the Prony series:

\[ G(t) = G_\infty + \sum_{i=1}^{l} G_i \exp\left(-\frac{t}{g_i}\right); \quad K(t) = K_\infty + \sum_{j=1}^{J} K_j \exp\left(-\frac{t}{k_j}\right). \tag{2.2.16} \]

Here, \( g_i (i = 1..I) \) and \( k_j (j = 1..J) \) are the deviatoric and volumetric relaxation times respectively; \( G_i (i = 1..I) \) and \( K_j (j = 1..J) \) are the corresponding moduli or weights, and \( G_\infty \) and \( K_\infty \) the long-term elastic shear and bulk moduli.

The deviatoric and dilatational parts of the effective stress are then found from equation (2.2.7) as follows:

\[
\begin{align*}
\tilde{s}(t) &= \tilde{s}_\infty(t) + \sum_{i=1}^{l} \tilde{s}_i(t) \\
\tilde{\sigma}_H(t) &= \tilde{\sigma}_H\infty(t) + \sum_{j=1}^{J} \tilde{\sigma}_H j(t)
\end{align*}
\tag{2.2.17}
\]

where

\[
\begin{align*}
\tilde{s}_\infty(t) &= 2G_\infty \xi^{ve}(t); \quad \tilde{s}_i(t) = 2G_i \int_{-\infty}^{t} \exp\left(\frac{\tau - t}{g_i}\right) \frac{\partial \xi^{ve}(\tau)}{\partial \tau} \, d\tau \\
\tilde{\sigma}_H\infty(t) &= 3K_\infty \xi_H^{ve}(t); \quad \tilde{\sigma}_H j(t) = 3K_j \int_{-\infty}^{t} \exp\left(\frac{\tau - t}{k_j}\right) \frac{\partial \xi_H^{ve}(\tau)}{\partial \tau} \, d\tau
\end{align*}
\tag{2.2.18}
\]
2.2 Proposed model

The strain tensor being also divided into deviatoric and dilatational parts:
\[ \varepsilon(t) = \varepsilon^{\text{dev}}(t) + \varepsilon^{\text{vel}}(t) \]

Using equations (2.2.17) and (2.2.18) with Prony series (2.2.16) (see Appendix B for details), a remarkably simple expression of the damage thermodynamic force \( Y \) (eq. 2.2.12) is found:
\[ Y = \frac{\hat{s}_{\infty} : \hat{s}_{\infty}}{4G_{\infty}} + \frac{(\hat{\sigma}_{H_{\infty}})^2}{2K_{\infty}} + \sum_{i=1}^{I} \frac{\hat{\sigma}_{i} : \hat{s}_{i}}{4G_{i}} + \sum_{j=1}^{J} \frac{(\hat{\sigma}_{H_{j}})^2}{2K_{j}} \]

Following almost the same procedure as for \( Y \), the expression of VE dissipation \( \phi^{\text{ve}} \) (eq. 2.2.14) is expressed by:
\[ \phi^{\text{ve}} = \frac{1}{4} \sum_{i=1}^{I} \frac{\hat{\sigma}_{i} : \hat{s}_{i}}{G_{i}g_{i}} + \frac{1}{2} \sum_{j=1}^{J} \frac{(\hat{\sigma}_{H_{j}})^2}{K_{j}k_{j}} \]

2.2.2 Evolution laws

In this section, the concepts of generalized potential and generalized standard materials are used (Chaboche, 1997) together with the rule of generalized normality expressed as:
\[ \dot{\varepsilon}^{\text{vp}} = \frac{\gamma}{\dot{\sigma}} \frac{\partial F}{\partial \varepsilon}, \dot{V} = \frac{\dot{\gamma}}{\dot{\sigma}} \frac{\partial F}{\partial A} \]

Here \( \gamma \) is a viscoplastic multiplier and the potential \( F \) is chosen as in (Lemaitre and Chaboche, 1994):
\[ F(\sigma, R, X, Y; D) = f(\sigma, R, X; D) + \frac{b}{2a} X : X + F_D(Y; D) \]

where \( f(\sigma, R, X; D) \) represents the viscoelastic domain if \( f < 0 \), and VP flow if \( f > 0 \) and \( F_D \) is the damage potential. The following expression for \( f \) is considered:
\[ f(\sigma, R, X; D) = (\hat{\sigma} - X)^{eq} - \sigma_Y - R(r) \]

Here \( \sigma_Y \) is the VE limit (which may depend on the strain rate) and \( (\hat{\sigma} - X)^{eq} \) is chosen as the Von Mises measure of \( (\hat{\sigma} - X) \):
\[ (\hat{\sigma} - X)^{eq} = \left[ \frac{3}{2}(\hat{s} - X) : (\hat{s} - X) \right]^{1/2} \]

Using (eq. 2.2.22), the following evolution equations are found:
\[ \dot{\varepsilon}^{\text{vp}} = \frac{\dot{\gamma}}{1 - D} \dot{N}, \dot{\alpha} = \dot{\gamma}(\dot{N} - \frac{b}{a} X), \dot{\gamma} = \dot{\gamma}, \dot{D} = \dot{\gamma} \frac{\partial F_D}{\partial \dot{Y}} \]

Where the following notation was introduced:
\[ \hat{N} \equiv \frac{\partial f}{\partial \sigma} = -\frac{\partial f}{\partial X} = \frac{3}{2} \frac{(\hat{s} - X)}{(\hat{\sigma} - X)^{eq}} \]
2.2 Proposed model

If the damage is inactive, the tensor $\tilde{N}$ is normal to the yield surface in the stress space. Since $\dot{\varepsilon}^{vp}, \tilde{N}$, and $X$ are deviatoric and $(\tilde{N} : \tilde{N} = 3/2)$, the accumulated viscoplastic strain rate $\dot{\gamma}$ is related to $\hat{\gamma}$ and $\hat{\tau}$ by:

$$\dot{\gamma} = \dot{\tau} = (1 - D)\hat{\gamma} ; \dot{\gamma} = \left(\frac{2}{3} \dot{\varepsilon}^{vp} : \dot{\varepsilon}^{vp}\right)^{1/2} \tag{2.2.28}$$

and it is defined by:

$$\begin{align*}
\dot{\gamma} &= 0 & \text{if } f \leq 0 \\
\dot{\gamma} &= g_v((\tilde{\sigma} - X)_{eq}, r) > 0 & \text{if } f > 0
\end{align*} \tag{2.2.29}$$

where $g_v$ is a viscoplastic function which could be expressed with a Norton power law for instance:

$$g_v = \frac{\sigma_Y}{\eta} \left(\frac{f}{\sigma_Y}\right)^m \tag{2.2.30}$$

The damage potential $F_D(Y; D)$ for ductile damage evolution is chosen as:

$$F_D(Y; D) = \frac{S}{s + 1} \left(\frac{Y}{S}\right)^{s+1} \frac{1}{1 - D} \tag{2.2.31}$$

which gives the Chaboche-Lemaitre damage evolution law (Lemaitre, 1985b) (see Fig. 2.3.1):

$$\begin{align*}
\dot{D} &= \left(\frac{Y}{S}\right)^s \dot{\gamma} \geq 0 & \text{if } p > p_D \\
\text{If } D &= D_c \rightarrow \text{crack initiation}
\end{align*} \tag{2.2.32}$$

where $p_D$ is a damage threshold, $D_c$ is a critical damage value and $s, S$ are material parameters. In this work, $p_D$ and $D_c$ are not considered as material constants, but they depend on the strain rate, which might be explained by the rate dependency of the failure mode. Note that in the damage fatigue model for metals of Lemaitre and Doghri (1994), $p_D$ and $D_c$ are not considered constant either. Once the strain-rate dependencies of $p_D$ and $D_c$ identified from uniaxial tests, one can either propose analytical functions or use interpolation between the discrete values to model those dependencies. If the model is implemented in FE code in order to calculate a complex structure with heterogeneous strain rates, the appropriate values of $p_D$ and $D_c$ may be found based on local values of the equivalent strain rates.

2.2.3 Summary set of constitutive equations

In summary, the proposed VEVPD model can be described by the following set of constitutive equations:

\[ \text{eqn} \]
Proposed model

\[
\begin{align*}
\varepsilon &= \varepsilon^e + \varepsilon^p \\
\mathbf{\sigma}(t) &= (1 - D(t)) \int_0^t \mathbf{C}^e(t - \eta) : \mathbf{\varepsilon}^e(\eta) \, d\eta, \\
\dot{\varepsilon}^p &= \frac{3}{2} \left( \mathbf{\dot{s}} - \mathbf{X} \right) \dot{p}, \\
\dot{\mathbf{X}} &= (1 - D)(a\dot{\varepsilon}^p - b\mathbf{X} \dot{p}), \\
\dot{\mathbf{r}} &= (1 - D)\dot{p} = g_v((\mathbf{\dot{\sigma}} - \mathbf{X})_{eq}, r) \geq 0, \text{ if } f > 0 \text{ otherwise } : \dot{r} = 0 \\
\dot{D} &= \left( \frac{Y}{S} \right)^s \dot{p} \geq 0 \text{ if } p > p_D \text{ until } D = D_c \rightarrow \text{ crack initiation} \\
Y &= \frac{\mathbf{\dot{s}}_{\infty} : \mathbf{\dot{s}}_{\infty}}{4G_{\infty}} + \frac{(\mathbf{\dot{\sigma}}_{H_{eq}})^2}{2K_{\infty}} + \frac{1}{4} \sum_{i=1}^{I} \frac{\mathbf{\dot{s}}_{i} : \mathbf{\dot{s}}_{i}}{G_{i}} + \frac{1}{2} \sum_{j=1}^{J} \frac{(\mathbf{\dot{\sigma}}_{H_{j}})^2}{K_{j}} \\
(2.2.33)
\end{align*}
\]

Note that eq.(2.2.33-b) relates the stress to the VP strain implicitly because the VE strain ($\varepsilon^e$) is found from the total strain ($\varepsilon$) which is usually given and the VP strain ($\varepsilon^p$) using eq.(2.2.33-a). Also the evolution of the damage variable ($D$) is function of the accumulated VP strain rate ($\dot{p}$), eq.(2.2.33-f), which is related to the VP strain ($\varepsilon^p$) rate, eq.(2.2.33-c). Figure 2.2.2, presents an illustration of the model in the case of a monotonic uniaxial tension loading.

The yield function in this case is reduced to:

\[
f = \mathbf{\sigma}_{11} - \frac{3}{2} X_{11} - \sigma_{Y} - R(r) \quad (2.2.34)
\]

Figure 2.2.2: Illustration of VEVPD model in the case of uniaxial monotonic tension loading
2.3 Numerical simulations and experimental validation

Several cases corresponding to different models, can be treated with the same proposed model, by setting appropriate values to some material parameters:

- The elasto-(Visco)Plastic-(Damaged) model is found when the shear and bulk relaxation times are taken to be infinite ($g_i \rightarrow +\infty$ and $k_j \rightarrow +\infty$),
- The (Visco)elasto-Plastic-(Damaged) model is found by setting plasticity to be rate-independent (for instance with Norton law (eq. 2.2.30), by making $\eta$ go to zero),
- Damage can be turned off by setting the damage threshold, $p_D$ to a very large positive value.
- Kinematic hardening can be turned off by setting $a = 0$ and $b = 0$.
- Kinematic hardening can be made linear by setting $b = 0$.
- Isotropic hardening can be turned off by choosing power law (eq. 2.2.11) and $k = 0$.
- Isotropic hardening can be made linear by choosing power law (eq. 2.2.11) and $n = 1$.
- Viscoelasticity can be turned off all together (and the model becomes purely VE) by setting the initial yield stress, $\sigma_y$, to a very large positive value.

2.3 Numerical simulations and experimental validation

In this section, predictions of the behavior of three thermoplastic polymers (Polypropylene, Nylon 101 and high-density polyethylene: HDPE) under various loading conditions are compared to some available experimental results in the literature. A numerical integration algorithm for the proposed VEVPD model was developed following the methods used in (Doghri, 1995; Simo and Hughes, 1998; Doghri, 2000; Miled et al., 2011). Based on a strain-driven procedure, for a generic time interval $[t_n, t_{n+1}]$, the values of the variables at $t_n$ are known and the total strain increment $\Delta \varepsilon$ is given. The algorithm computes the variables at time $t_{n+1}$. For the proposed model coupling VE, VP, damage and nonlinear kinematic hardening, the developed algorithm involves lengthy derivations, which are summarized in Appendix B.

2.3.1 Material parameters identification

If the material is considered to be virgin before applying the loading, the behavior is assumed to be VE-VP and the damage effect is neglected. As discussed by Miled et al. (2011) the material parameters should be identified based on separate experiments.
2.3 Numerical simulations and experimental validation

The dynamic response of a sample subjected to oscillatory excitation (Lakes, 1999) under different frequencies in uniaxial tension/compression and in simple shear or in torsion allow to determine the relaxation times and moduli in the Prony series of $G(t)$ and $K(t)$. The VP material parameters are found by loading the material above and near the yield point based on uniaxial tensile tests. In uniaxial response, the stress is independent of the Poisson’s ratio, and the VE Young’s modulus may be described by a Prony series:

$$E(t) = E_{\infty} + \sum_{i=1}^{I} E_i \exp\left(-\frac{t}{\tau_i}\right)$$

(2.3.1)

where the parameters $E_{\infty}$, $E_i$ and $\tau_i$ may be identified using the procedure presented in Appendix C.

Poisson’s ratio (PR) for VE thermoplastic polymers, is proven to be time, stress and thermal expansion dependent, which makes PR values determined from a uniaxial test not applicable to other uniaxial loadings with different time histories or to multiaxial loadings and thermal expansions (Hilton and Yi, 1998; Tschoegl et al., 2002; Lakes and Wineman, 2006). Rigorously, PR is not a material parameter for VE thermoplastics. The use of shear and bulk time functions, expressed using Prony series determined directly from experiments is more appropriate to model the multiaxial aspects of material behavior. However, if the only available experimental data are uniaxial tests, then an estimate of the shear and bulk moduli may be found, assuming a constant Poisson’s ratio:

$$\begin{align*}
G_\infty &= \frac{E_\infty}{2(1+\nu)} ; G_i = \frac{E_i}{2(1+\nu)} ; \quad g_i = \frac{\tau_i E_i}{G_i} \quad \text{(no sum)} \\
K_\infty &= \frac{3(1-2\nu)}{E_\infty} ; K_i = \frac{3(1-2\nu)}{E_i} ; \quad k_i = \frac{\tau_i E_i}{K_i}
\end{align*}$$

(2.3.2)

Similar assumptions about Poisson’s ratio, were made by Miled et al. (2011) for HDPE, and by Kästner et al. (2012) for Polypropylene. Once the VE and the VP parameters are computed, the material damage parameters ($S, s, D, D_c$) are determined using cyclic tensile loading. The change of the shape of the stress curve under unloading/reloading could be interpreted as a tracer of the damage effect as shown in figure 2.3.1. The critical value of $(D_c \leq 1)$ corresponds to the abrupt decrease of the stress (i.e. the material is no longer able to carry the applied loading).
2.3 Numerical simulations and experimental validation

The material parameters \((S, s)\), representing the evolution of the damage law, are found by reverse analysis. Since the Lemaitre damage law was developed initially for metals, some conditions on parameters \((S, s)\) have been made to fit more with metals, such as \((s \geq 0.1)\). For thermoplastic polymers the evolution of the damage is very different from that for metals (Detrez et al., 2011). Then to capture the damage evolution for polymers, the parameter \((s)\) may be negative (see the curve of \(D\) as function of \(p\), in figure 2.3.1). This allows to model damage saturation as exhibited by the experimental investigation of (Detrez et al., 2011).

For monotonic tensile loading, or for few cycles of loading, the effect of kinematic hardening on the response of the material could be neglected. Otherwise, parameters \((a, b)\) have to be found to capture the influence of the cyclic loading on the yield surface.

### 2.3.2 Monotonic tensile loadings under different strain rates

Kästner et al. (2012) published experimental results on Polypropylene under tensile monotonic loading for three strain rates \((1.5 \times 10^{-2}, 1.5 \times 10^{-3}, 1.5 \times 10^{-4})\) s\(^{-1}\) until failure. The identified parameters are listed in table 2.1. The material is assumed to be virgin at the beginning of loading and behaves as a VE-VP material without damage; numerical predictions are presented in figure 2.3.2 compared to experiments under different strain rates.
2.3 Numerical simulations and experimental validation

Figure 2.3.2: Polypropylene response under tensile loading with different strain rates. Fitted material parameters are listed in table 2.1. Symbols stand for experimental results from Kästner et al. (2012) and lines for numerical simulations with VEVPD model.

For larger strains, Kästner et al. (2012) reported experimental results in terms of nominal stress and strain. For nominal strains smaller than 20%, it is unclear whether necking of the specimens was observed or not. Since Kästner et al. (2012) supposed material incompressibility, we made the same assumption and computed true stress and strain according to the following formulate (in the uniaxial case):

\[
\begin{align*}
\sigma_{11T} &= \sigma_{11N} (1 + \varepsilon_{11N}) \\
\varepsilon_{11T} &= \ln(1 + \varepsilon_{11N})
\end{align*}
\]  

(2.3.3)

where \(\sigma_{11T}\) and \(\sigma_{11N}\) are true and nominal uniaxial stresses, respectively. \(\varepsilon_{11T}\) and \(\varepsilon_{11N}\) are true and nominal strains, respectively.

If there is necking, then the above method for calculating the constitutive response is too approximate, and one has to use correction models (eg. Bridgman, 1944) or finite element analysis of the whole specimens.

In this work, based on eqs. 2.3.3 the experimental data of Kästner et al. (2012) were transformed into true stress vs. true strain curves, and the proposed VEVPD model was identified against them - see figure 2.3.3. However, if there is necking, then the results of figure 2.3.3 do not correspond to the material’s constitutive response, which may not show any softening in terms of true stress. The proposed model captures the strain rate dependency and the material softening. As indicated in section 2.3.1, the values of \(p_D\) and \(D_c\) are not material constants, but depend on the strain rate.
2.3 Numerical simulations and experimental validation

Figure 2.3.3: Polypropylene response under tensile loading with different strain rates: Fitted material parameters are listed in table 2.1. (a) Axial true stress vs. axial true strain, (b) Axial nominal stress vs. axial nominal strain. Symbols stands for experimental results from Kästner et al. (2012) and lines for numerical simulations with the proposed VEVPD model.
2.3 Numerical simulations and experimental validation

Viscoelastic parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Young’s modulus</td>
<td>$E_0 = 1410$ MPa</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$\nu = 0.40$</td>
</tr>
<tr>
<td>$E_i$ (MPa)</td>
<td>$\tau_i$ (s)</td>
</tr>
<tr>
<td>700</td>
<td>250</td>
</tr>
<tr>
<td>240</td>
<td>40</td>
</tr>
<tr>
<td>130</td>
<td>2</td>
</tr>
</tbody>
</table>

Viscoplastic and Damage parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial yield stress</td>
<td>$\sigma_y = 10$ MPa</td>
</tr>
<tr>
<td>Isotropic hardening</td>
<td>$k = 65$ MPa</td>
</tr>
<tr>
<td>$n$</td>
<td>$n = 0.39$</td>
</tr>
<tr>
<td>Viscoplastic function</td>
<td>$\eta = 120$ MPa.s</td>
</tr>
<tr>
<td>$m$</td>
<td>$m = 9$</td>
</tr>
<tr>
<td>Damage parameters</td>
<td></td>
</tr>
<tr>
<td>$S = 0.09$ MPa</td>
<td></td>
</tr>
<tr>
<td>$P_D(1.5 \times 10^{-2}) = 0.035$</td>
<td>$D_{c}(1.5 \times 10^{-2}) = 20%$</td>
</tr>
<tr>
<td>$P_D(1.5 \times 10^{-3}) = 0.015$</td>
<td>$D_{c}(1.5 \times 10^{-3}) = 25%$</td>
</tr>
<tr>
<td>$P_D(1.5 \times 10^{-4}) = 0.00$</td>
<td>$D_{c}(1.5 \times 10^{-4}) = 30%$</td>
</tr>
</tbody>
</table>

Table 2.1: Constitutive model parameters for Polypropylene identified from experimental data of Kästner et al. (2012)

2.3.3 Multiaxial loadings under different strain rates

In this section the proposed model is used to simulate the behavior of Nylon 101 under three loading conditions: tension, torsion and combined tension-torsion. The experimental results are due to Farrokh and Khan (2010), the incompressibility of this material was checked by Khan and Farrokh (2006). The experimental tests were carried under various equivalent strain rates, defined as follows:

$$\varepsilon_{eq} = \left(\varepsilon_{11}^2 + \left(\frac{\gamma_{12}}{\sqrt{3}}\right)^2\right)^{1/2} \quad (2.3.4)$$

where $\varepsilon_{11}$ is the axial strain in direction 1 and $\gamma_{12}$ is the engineering shear strain.

As a first assumption, it is considered that Nylon 101 obeys an elastoviscoelastic (EVP) version of the proposed model. Parameter values are in table 2.2 (with damage disabled), fitted from the tensile tests under different strain rates. Figure 2.3.4 presents the numerical simulation of uniaxial tension compared to the experimental results. Next, the model in its EVP version, was used to predict the material behavior in the case of torsion and combined tension-torsion. The results are shown in Figs 2.3.5 and 2.3.6 (a) and (b). Figures 2.3.4 to 2.3.6 show that the EVP model is able to capture strain rate effects for the different loading cases. However for large strain rates the EVP model overestimates the stress values.
2.3 Numerical simulations and experimental validation

Figure 2.3.4: Nylon101 response under uniaxial tension with different strain rates. Symbols stand for experimental results from Farrokh and Khan (2010) and solid lines for numerical simulations with the EVP version of the proposed model. Material parameters are listed in table 2.2.

Figure 2.3.5: Predictions of Nylon101 response under pure torsion with different equivalent strain rates. Symbols stand for experimental results from Farrokh and Khan (2010) and solid lines for numerical simulations with the EVP version of the proposed model. Material parameters are listed in table 2.2.
Figure 2.3.6: Predictions of Nylon101 response under combined tension-torsion loading with different equivalent strain rates: (a) Axial true stress vs. axial true strain, (b) Shear true stress vs. shear strain. Symbols stand for experimental results from Farrokh and Khan (2010) and solid lines for numerical simulations with the EVP version of the proposed model. Material parameters are listed in table 2.2.

For both cases of torsion and combined tension-torsion, one can notice a slight difference between the experimental data and the numerical simulations in the linear part of the material behavior. This is a consequence of assuming that the shear stress components related to torsion are uniform, which is not generally the case when a part is submitted to a torsion loading except for
2.3 Numerical simulations and experimental validation

particular cases of specimen geometries. In the torsion experiments of Farrokh and Khan (2010), the authors employed hollow cylindrical specimens (external diameter is 1.5 cm and internal diameter is 1.3 cm). The specimen may be considered as a thin circular tube (cf. more detail about the stresses within this specimen particular geometry under a torsion loading in the book (Doghri, 2000, section 4.12.8)). The stresses are assumed to be uniform within the material, in order to have a fast evaluation of the model capabilities under multiaxial loadings.

In a second modeling attempt, weak damage effects were introduced, thus the EVP-D version of the proposed model was used. Parameter values are listed in table 2.2, fitted from tensile tests under various strain rates. The results are presented in figures 2.3.7 and 2.3.8. An improvement of stress estimation is seen although for the highest strain rate ($\dot{\varepsilon}_{eq} = 1s^{-1}$) the model still overestimates the stress. This could be explained by the model not taking into account self-heating which may become important at large strain rates.

![Figure 2.3.7: Nylon101 response under uniaxial tension with different strain rates. Symbols stand for experimental results from Farrokh and Khan (2010) and solid lines for numerical simulations with the EVP-D version of the proposed model. Material parameters are listed in table 2.2](image)
2.3 Numerical simulations and experimental validation

### Elastic parameters

- Young’s modulus \( E_0 = 3700 \text{ MPa} \)
- Poisson’s ratio \( \nu = 0.49 \)

### Viscoplastic and damage parameters

- Yield stress \( \sigma_y = 36 \text{ MPa} \)
- Isotropic hardening \( k = 75 \text{ MPa} \), \( n = 0.25 \)
- Viscoplastic function \( \eta = 3600 \text{ MPa.s} \), \( m = 9 \)
- Damage parameters \( S = 0.06 \text{ MPa} \), \( s = 0.01 \)

Table 2.2: Constitutive model parameters for Nylon 101 identified from experimental tensile tests of Farrokh and Khan (2010)

![Graph showing prediction of Nylon101 response under pure torsion loading with different strain rates. Symbols stand for experimental results from Farrokh and Khan (2010) and solid lines for numerical simulations with the EVPD version of proposed model. Material parameters are listed in table 2.2.](image)

**Figure 2.3.8:** Prediction of Nylon101 response under pure torsion loading with different strain rates. Symbols stand for experimental results from Farrokh and Khan (2010) and solid lines for numerical simulations with the EVPD version of proposed model. Material parameters are listed in table 2.2.

**2.3.4 Cyclic loadings**

Due to the rather complex response of thermoplastic polymers under cyclic loadings, good predictions are challenging. The proposed model was used to predict the behavior of high-density polyethylene (HDPE) under cyclic loading. Experimental results from Zhang and Moore (1997) are strain controlled, the successive values of the prescribed elongation are given in table 2.4. Figures 2.3.9 and 2.3.10 present numerical predictions compared to experiments in case of cyclic loading at a strain rate \( (\pm 10^{-4}s^{-1}) \). Material parameters are listed in table 2.3. The VEVPD model gives better predictions compared to those
2.3 Numerical simulations and experimental validation

of the VE-VP model of Miled et al. (2011) which could be obtained as a particular version of the proposed model and those of the uniaxial linear VE-VP model of Chehab and Moore (2004) developed based on a multi-Kelvin linear viscoelastic model of Moore and Hu (1996). In figure 2.3.10, the models predict negative stresses while the experimental stresses remain tensile. This is due to an insufficient modeling of VE unloading. However, the proposed VEVPD performs better than the other two, as can be seen by comparing figures 2.3.9 (b) and 2.3.9(a).

<table>
<thead>
<tr>
<th>Viscoelastic parameters</th>
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</tr>
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<tbody>
<tr>
<td>Initial Young’s modulus</td>
<td>$E_0 = 1500$ MPa</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$\nu = 0.3$</td>
</tr>
<tr>
<td>$E_i$ (MPa)</td>
<td>$\tau_i(s)$</td>
</tr>
<tr>
<td>796</td>
<td>120</td>
</tr>
<tr>
<td>349</td>
<td>20</td>
</tr>
<tr>
<td>73</td>
<td>5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Viscoplastic and Damage parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Yield stress</td>
<td>$\sigma_y = 10$ MPa</td>
</tr>
<tr>
<td>Isotropic hardening</td>
<td>$k = 42$ MPa $n = 0.39$</td>
</tr>
<tr>
<td>Viscoplastic function</td>
<td>$\eta = 106$ MPa.s $m = 7$</td>
</tr>
<tr>
<td>Damage parameters (model type II)</td>
<td>$S = 1.2$ MPa $s = -1.4$</td>
</tr>
</tbody>
</table>

Table 2.3: Constitutive model parameters for HDPE identified from experimental data of Zhang and Moore (1997) for the VEVPD model.

<table>
<thead>
<tr>
<th>Load1</th>
<th>Unload1</th>
<th>Load2</th>
<th>Unload 2</th>
<th>Load3</th>
<th>Unload 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strain</td>
<td>0.028</td>
<td>0.011</td>
<td>0.05</td>
<td>0.031</td>
<td>0.071</td>
</tr>
</tbody>
</table>

Table 2.4: History of loading 1 of HDPE at a strain rate$(\pm 10^{-4} s^{-1})$
2.3 Numerical simulations and experimental validation

Figure 2.3.9: behavior of HDPE under cyclic tensile loading at a strain rate of $(\pm 10^{-4}\text{s}^{-1})$: (a) Numerical simulations using VE-VP model of Miled et al. (2011) and the uniaxial linear VE-VP model of Chehab and Moore (2004); (b) Using the proposed VEVP-D model. Fitted material parameters are listed in table 2.3.

The dissipated energy $\phi$ is depicted in figure 2.3.11, where one can see the effect of the cyclic loading on the value of the energy. The value of the dissipated energy increases during unloading due to the viscoelastic dissipation.
2.3 Numerical simulations and experimental validation

\[ \phi^{\text{ej}}. \]

Figure 2.3.10: behavior of HDPE under uniaxial tensile compression test at a strain rate of \((\pm 10^{-4}\text{s}^{-1})\). Fitted material parameters are listed in table 2.3. Dots stand for experimental results from Zhang and Moore (1997), lines for predictions using the proposed VEVPD model, VE-VP model of Miled et al. (2011) and the uniaxial linear VE-VP model of Chehab and Moore (2004).

Figure 2.3.11: Dissipated energies within the HDPE material during the two loading histories of Figs. 2.3.9 and 2.3.10
2.3 Numerical simulations and experimental validation

For mechanical testing of materials under fatigue loading in order to determine their lifetime, the standard tests are mostly carried either with strain or stress control. Some predictions of the VEVPD model in the case of strain controlled tests are presented hereafter. Since it is very difficult to find detailed experimental data on fatigue of thermoplastic polymers in literature, some numerical simulations were made using the already identified material parameters for Polypropylene and the obtained trends were compared to those in the literature.

Under strain-controlled tests on polymers, the peak stresses usually decrease from one cycle to another or remain almost constant. This could be explained by a complex phenomenon combining viscosity and plastic yielding within the material. The effect of viscosity could lead to a behavior similar to the one under relaxation if the mean applied strain is constant. Figure 2.3.12 presents the behavior of Polypropylene under constant maximum and minimum controlled strain using the VEVPD model; notice the similar trend between the experimental results on the right of figure 2.3.12 and the numerical predictions on the left.

When plastic yielding occurs, the plastic accumulation increases under cyclic loading and the value of the isotropic hardening also increases. So the peak stress increases from cycle to cycle, which is the opposite of the experimental trends. Damage and kinematic hardening are necessary to model the softening and the change of the plastic yield surface’s position in the stress space, respectively. Figure 2.3.13 depicts the prediction of maximum uniaxial stress evolution within the Polypropylene material using the VEVPD model. The maximum uniaxial stress value decreases from one cycle to another until material failure or remain almost constant. If the values of the applied strain induce a stress state inside of the yield surface (i.e. $f < 0$), the material remains purely viscoelastic and no plastic strains evolve within the material, then the peak stresses remain almost constant. In experimental literature, similar tendencies are well known for polymeric materials (Lesser, 1995) and for polymeric
2.3 Numerical simulations and experimental validation

matrix composite material (Bellenger et al., 2006). The difference is that the material fails even when the peak stress remain constant, after a large number of cycles. These two tendencies may be associated to low cycle fatigue (LCF) and high cycle fatigue (HCF).

![Figure 2.3.13: Prediction of Polypropylene response under constant maximum and minimum controlled strain for different values of maximum strain at strain rate (\(\dot{\varepsilon} = \pm 0.00015 \text{s}^{-1}\)) and with a loading ratio \(\epsilon_{11\text{min}}/\epsilon_{11\text{max}} = 0\). Material parameters are in table 2.1.](image)

Figure 2.3.13: Prediction of Polypropylene response under constant maximum and minimum controlled strain for different values of maximum strain at strain rate (\(\dot{\varepsilon} = \pm 0.00015 \text{s}^{-1}\)) and with a loading ratio \(\epsilon_{11\text{min}}/\epsilon_{11\text{max}} = 0\). Material parameters are in table 2.1.

2.3.5 Effect of kinematic hardening

The effect of kinematic hardening was neglected in all the previous simulations, and was deactivated in the model. In this section, the focus is on kinematic hardening and its effect on the material behavior. In order to show its interaction with damage, a parametric study is performed with and without the presence of damage, using the parameters \(a\) and \(b\) of the kinematic hardening law. The identified parameters for HDPE, listed in table 2.3, are used.

Figure 2.3.14 shows the effect of the variation of the parameter \(a\) of kinematic hardening law in the case of \((b = 0)\) and deactivated damage. In this case the kinematic hardening is linear. Figure 2.3.15 shows the effect of the parameter \(b\) variation for constant value of \(a\) (taken equal to 300 MPa) also with deactivated damage. The effect of variation of those parameters is mainly important under the loading however no effect is noticed on the slope under unloading. Those tendencies are due to the fact that the loading is characterized by a VP behavior and because the plastic deformation evolves only during the VP transformation, the value of the kinematic hardening is also evolving, however for unloading the behavior is mainly VE, and the value of the kinematic hardening is constant during this transformation and has no effect on

47
2.3 Numerical simulations and experimental validation

the viscoelastic parameters.

(a)

\[
\begin{array}{c}
\text{Stress (} \sigma_{11} \text{)} [\text{MPa}] \\
0 & 5 & 10 & 15 & 20 & 25 & 30 \\
\hline
\text{Strain (} \varepsilon_{11} \text{)} [\%] & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11
\end{array}
\]

(b)

\[
\begin{array}{c}
\text{Plastic accumulation (} p \text{)} [\%] \\
0 & 0.2 & 0.4 & 0.6 \\
\hline
\text{Strain } \varepsilon_{11} [\%] & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11
\end{array}
\]

Figure 2.3.14: Effect of variation of the parameter \( a \) on the stress strain curve (a) and on plastic accumulation (b) for HDPE, in the case of linear kinematic hardening law \((b = 0)\) and deactivated damage.
2.3 Numerical simulations and experimental validation

Figure 2.3.15: Effect of variation of the parameter $b$ on the stress strain curve (a) and on plastic accumulation (b) for HDPE, in the case of $a = 300$ and deactivated damage.

Similar analyses to the previous ones, are performed in the case of activated damage for various value of $a$ and $b$, the results are plotted respectively in figures 2.3.16 and 2.3.17. The effect of kinematic hardening parameters variation under loading is similar to the one in previous simulations, but unlike the case of deactivated damage, this variation has an effect on the material behavior under unloading. The effect is due to a different evolution of the plastic accumulation during the loading. The plastic accumulation evolution (cf. figures 2.3.16.b and 2.3.17.b ) is related to the damage evolution (cf. figure 2.3.16.c and 2.3.17.c ), thus the value of the damage during the unloading is different because of kinematic hardening parameters variation.
2.3 Numerical simulations and experimental validation

Figure 2.3.16: Effect of variation of the parameter $a$ on the plastic accumulation for HDPE, in the case of linear kinematic hardening law ($b = 0$) and activated damage.
2.3 Numerical simulations and experimental validation

Figure 2.3.17: Effect of variation of the parameter $b$ on the stress strain curve for HDPE, in the case of of value of $a = 300$ and activated damage.
2.4 Discussion and possible enhancements

The proposed VEVPD model was able to reproduce with good accuracy various experimental data from the literature. For Polypropylene, the stress-strain curves in uniaxial tension for different strain rates up to failure were simulated with good accuracy (Figs 2.3.2 and 2.3.3). For Nylon 101 under multiaxial loadings, the simulations of the model without and with damage were presented. The results are satisfactory, especially when the model includes even a weak damage evolution. However, for high strain rates, the proposed model overestimates the stress, probably because it does not take into account self-heating.

For HDPE under different unloading/reloading loops, the predictions were also good (Figs 2.3.9(a) and (b), and Fig.2.3.10). For Polypropylene under several strain-controlled cycles, the experimentally-observed trend for the maximum stress is correctly predicted (Fig.2.3.12). The model seems also able to model low cycle fatigue (Fig.2.3.13). In summary, the proposed model provides a good framework for modeling the deformation and progressive damage of thermoplastic polymers under various loading histories, and up to failure. Some improvement discussed hereafter can only enhance the predictive capabilities of the proposed VEVPD model.

For thermoplastic polymers, the crystallization condition may strongly influence their behavior (eg. Brooks et al., 1999; Detrez et al., 2011). Many studies associated damage to the amorphous phase especially under small strain condition, which could explain the softening phenomena. The material could fail after this softening under small strains for polymer type II (figure 2.4.1), such as Polypropylene considered in section 3, or the loading may still be carried with the crystalline part until the deformations reach large values (polymer type I in figure 2.4.1). The proposed VEVPD model can be used to predict the behavior of polymer type II via the damage variable. For the behavior of type I of thermoplastic polymers, a finite strain formulation of the model should give theoretically more justified and better predictions (eg. Holmes and Loughran, 2010; Peric and Dettmer, 2003).

In the case of fatigue loading, the model seems to be able to reproduce some experimentally known tendencies. However it is limited to low cycle mechanical fatigue, under small frequencies, since self-heating effect under higher frequencies can be important (Lesser, 1995). For high cycle fatigue (HCF) plastic yielding is localized and its effect is not visible at macroscale. Therefore, macroscale models, such as the present one, are limited to low cycle fatigue (LCF). In the proposed model, the damage does not evolve in pure VE transformations, it increases only if VP strains evolve.

Improvements are needed in order to better capture unloading (as in figures 2.3.9and 2.3.10), reloading in compression, and general cyclic tension-compression loads. In this regard, nonlinear instead of linear viscoelasticity can also be helpful.

The effect of hydrostatic pressure on polymers is important. Since the presented model is using the Von Mises yield criterion this phenomena is not well taken into account, although the damage law is sensitive to the hydrostatic stress, but it still not enough to fully capture the pressure effect on the
2.5 Conclusions

material behavior. To overcome this limitation a generalized Drucker-Prager criterion could be used, which will mainly involve important modifications to the numerical algorithm.

![Graph of Polymer Types I and II](image)

Figure 2.4.1: Illustration of type of behavior of polymers under tensile loading

2.5 Conclusions

In this chapter an original constitutive model coupling progressive damage, viscoelasticity and viscoplasticity was proposed for thermoplastic polymers under arbitrary loadings. The model is written within the framework of the thermodynamics of irreversible processes. It supposes a decomposition of the total strain into VE and VP parts. The undamaged Cauchy stress is a functional of the VE strain history through Boltzmann’s integral. Time dependent bulk and shear moduli obey general Prony series. The VP response combines nonlinear isotropic and kinematic hardenings. The evolution of the ductile damage is linked to that of VP strains. Closed form and simple expressions of the strain energy release rate and various dissipation contributions are found. Numerical predictions were validated against experimental tests on polymers under various loadings. Tests on Polypropylene and HDPE included monotonic tension under different strain rates up to failure, tensile load with several unloading/reloading loops, and low cycle fatigue. Experimental results on Nylon 101 were also reproduced, including tension, torsion and combined tension-torsion for strain rates ranging from low to high. In all cases, good agreement between model predictions and experimental results was found. The model could be improved following the suggestions presented in the discussion section. Possible enhancements involve a finite strain formulation, generalized Drucker-Prager pressure-dependent yield criterion, nonlinear viscoelasticity and thermal coupling.
Chapter 3

Mean field homogenization of viscoelastic viscoplastic damaged composites

All materials are heterogeneous at a given scale. Most modeling approaches start by assuming that the material is homogeneous or not based on macroscopic observations. Indeed, when the material is subjected to different types of loadings, the effect of its heterogeneity at lower scale may have an influence on its macroscopic response. Composite materials are a relevant example, for instance SFRTPs seem to be homogeneous at macroscale, but at microscopic scale they have a very complicated microstructure (cf. figure 1.2.3 for the case of SGFRPA66) causing the anisotropic behavior at macroscale. Multiscale modeling approaches have proven their efficiency for different kinds of heterogeneous materials and solids. For composite materials in a broad sense, two main categories of multiscale modeling approaches are usually distinguished. Firstly, there are the full field or direct methods, the most known being: finite element analysis, asymptotic homogenization, generalized method of cells, and fast fourier transform. Secondly, there are the mean-field homogenization methods. A comprehensive overview may be found in the book of Nemat-Nasser and Hori (1999). Mean field homogenization (MFH) is one of the methods aiming at estimating the overall behavior of multiphase composites, based on their microstructure. The specificity of MFH is to not perform a full field computation of a representative volume element (RVE), and to predict the overall response based on assumptions about the mean interaction between different phases. The MFH method is chosen to be employed in order to solve the studied problems, due to its proven efficiency during the last few decades. A brief review about the different MFH techniques is given in the first section of this chapter. The second section is devoted to presenting a proposed MFH model for two phase VEVPD composites where both matrix and inclusions have VEVPD behavior. Some numerical simulations using the proposed MFH model and possible enhancements are given in sections 3.4 and 3.5 respectively. The developed model was
employed in order to predict the behavior of TPs and SFRTPs mainly subjected to fatigue loadings (cf. chapters 4 and 5).

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3.1 Basic concepts about multiscale approaches

All multiscale approaches require to have a good knowledge about the material heterogeneity at a relevant scale, usually called microstructure. The more accurate is the knowledge of the microstructure, the better is the prediction of those approaches. The concept of a representative volume element (RVE) is usually employed, in order to represent the material microstructure and its heterogeneity at a given material point in a continuum mechanics sense. Different scales are then considered: the macroscale: the scale of the studied part and the mesoscale: the scale of the RVE (cf. figure 3.1.1).

Figure 3.1.1: Scale separation and characteristic length scales

An RVE has to respect the following conditions (Nemat-Nasser and Hori, 1999):

- \( l \ll L \): The size of the RVE \( l \) is much smaller than the one of the part \( L \),
- \( d \ll l \): Characteristic size of the heterogeneity \( d \) must be much smaller than the size of the RVE \( l \),
- \( d_0 \ll d \): The lower length bound \( d_0 \) under which continuum mechanics is no more valid should be much smaller then \( d \).
- \( l \ll \lambda \): The size of the RVE \( l \) is much smaller than the fluctuation length \( \lambda \) of a macroscopic deformation. Generally this condition is well satisfied, expect for cases such as localization of deformation and small wave length.

One of the important issues faced when employing an RVE is that of the boundary conditions. Generally, the loading is applied on the external RVE surface from which also the RVE average response is obtained. The loading may be controlled by an applied stress or strain. Using the Gauss theorem and classical definition of the strain \( \varepsilon \) and displacement \( u \) relation as well as the
3.1 Basic concepts about multiscale approaches

assumption of neglecting body forces \((\nabla \sigma = 0)\), the average of strain and stress\(^1\) can be defined as follows:

\[
\langle \varepsilon_{ij} (x) \rangle = \frac{1}{V} \int_{\omega} \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) dV = \frac{1}{2V} \int_{\partial \omega} (u_i n_j + u_j n_i) dA \tag{3.1.1}
\]

\[
\langle \sigma_{ij} (x) \rangle = \frac{1}{V} \int_{\omega} \frac{\partial (\sigma_{ik} x_j)}{\partial x_k} dV = \frac{1}{V} \int_{\partial \omega} t_i x_j dA \tag{3.1.2}
\]

where \(x\) is the position vector in a reference frame related to the RVE \(\omega\), defined by a volume \(V\) and a boundary \(\partial \omega\). \(t\) is a stress vector parallel to the normal unit vector \(n\) of the boundary \(\partial \omega\).

The most common used boundary conditions are linear displacement, uniform traction and periodic boundary conditions. For a relatively small size RVE, the periodic boundary condition gives closer results than the others boundary conditions, however for larger sizes all the listed methods gives good results, according to several works (e.g. Jiang et al., 2001; Kanit et al., 2003) (cf. figure 3.1.2).

Contrary to the full-field methods, mean-field homogenization methods aim at predicting the behavior of the whole RVE without computing the local fields. It is based on relating the mean values of the different fields in each phase of the RVE, based on assumed interaction laws between them. The full-field methods give a better approximation of the real solution compared to the mean-field method, however they are several orders of magnitude computationally more expensive than MFH. MFH techniques were applied to the case of linear and

\(^1\)Volume average value over the RVE of a field \(f\), is expressed as: \(\langle f (x) \rangle_\omega = \frac{1}{V} \int_{\omega} f (x) dV\)

Figure 3.1.2: (a) Several microstructural cells of different sizes. (b) Convergence of the apparent properties to the effective values with increasing microstructural cell sizes for different types of boundary conditions (From course on micromechanics in Eindhoven University of Technology, 2012)
3.2 Review of MFH techniques

The Mean Field Homogenization (MFH) techniques were developed for several types of constituent behavior, linear and nonlinear ones. They were initially developed for linear materials with aligned and identical inclusions, and later extended to nonlinear materials with more complex microstructure. The main advantage of the MFH techniques is the considerable reduction of computation time compared to full-field methods such as FE. For several material cases, they allow to obtain a very accurate prediction, especially in the linear elastic regime.

The problem of a linear two phase composite was studied based on classical results found in the last century, which were extended to the nonlinear regime in the last decades. In the following, several techniques of MFH employed in solving the problem of composites composed of two phases having a linear behavior is presented in the sub-section 3.2.1 and the case of nonlinear composites is presented in sub-section 3.2.2. A review of MFH techniques extensions for multiphase and misaligned inclusions reinforced composites is given in sub-section 3.2.3.

3.2.1 MFH techniques for linear composites

3.2.1.1 MFH of isothermal linear elastic composites

All phases are assumed to be homogeneous and elastic. Based on the interaction tensor concept, or concentration tensor as known in the literature, the interaction between the phases is modeled. The theory is developed for a non-limited number of phases. However, in practice, it is usually applied for two phase composites with identical inclusions, where only one concentration tensor is needed. The mean field theory employs an average value over the volume of the studied fields (stress or strain).

For a two phase composite with matrix and inclusions phases occupying domains $\omega_0$ and $\omega_1$, respectively, the volume average value of a field ($\cdot$) over the whole domain $(\omega = \omega_0 \cup \omega_1)$ is defined by:

$$\langle \cdot \rangle_{\omega} = v_1 \langle \cdot \rangle_{\omega_1} + (1-v_1) \langle \cdot \rangle_{\omega_0} \quad (3.2.1)$$

where $v_1$ is the volume fraction of the phase occupying $\omega_1$. According to MFH method, the average value of strains over $\omega_1$ is related to the one over $\omega_0$ by a strain concentration tensor $\mathbb{B}^c$ and to the macro-strain by another strain concentration tensor $\mathbb{A}^c$:

$$\langle \varepsilon \rangle_{\omega_1} = \mathbb{A}^c : \langle \varepsilon \rangle_{\omega} = \mathbb{B}^c : \langle \varepsilon \rangle_{\omega_0} \quad (3.2.2)$$

Using the equation (3.2.1), $\mathbb{A}^c$ can be expressed as function of $\mathbb{B}^c$ as:
3.2 Review of MFH techniques

\[
A^e = B^e : [v_1 B^e + v_0 I]^{-1} = [v_1 I + v_0 B^e]^{-1}
\]  
(3.2.3)

The relation of the average strain and the average stress in each phase is defined by Hooke’s law via a fourth order elastic operator \( C_{\omega_i} \), and expressed as:

\[
(\sigma)_{\omega_i} = C_{\omega_i} : (\epsilon)_{\omega_i}, \quad i \in \{0, 1\}, \text{ no sum}
\]  
(3.2.4)

The macro-stress \( \langle \sigma \rangle_{\omega} \) and the macro-strain \( \langle \epsilon \rangle_{\omega} \) over the RVE, are related by a similar relation using a so-called elastic stiffness operator \( C_{\omega} \). The expression of \( C_{\omega} \) is obtained using the above relations as follows:

\[
C_{\omega} = [v_1 C_{\omega_1} : B^e + (1 - v_1) C_{\omega_0}] : [v_1 B^e + (1 - v_1) I]^{-1}
\]  
(3.2.5)

Hence, the problem is reduced to finding the strain concentration tensors \( A^e \) or \( B^e \). Hereafter, some approaches are presented.

Simple homogenization schemes

Voigt (1889) and Reuss (1929) models are simple homogenization schemes, that give good results in particular cases only. However, they provide bounds for the real composite behavior.

- The Voigt model assumes a uniform strain in the RVE \( (B^e = I) \), the homogenized elastic operator \( C_{\omega} \) is given as:
  
  \[
  C_{\omega} = C_{\omega_1}^{Voigt} = v_1 C_{\omega_1} + (1 - v_1) C_{\omega_0}
  \]  
  (3.2.6)

- The Reuss model assumes a uniform stress in the RVE \( (B^e = C^{-1}_{\omega_1} : C_{\omega_0}) \), the homogenized tangent operator \( C_{\omega} \) is obtained as:
  
  \[
  C_{\omega} = C_{\omega_1}^{Reuss} = [v_1 C_{\omega_1}^{-1} + (1 - v_1) C_{\omega_0}^{-1}]^{-1}
  \]  
  (3.2.7)

Homogenization schemes based on isolated inclusion problem

Based on Eshelby’s results (Eshelby, 1957), other estimations of the concentration tensor are derived. Eshelby solved the problem of a single inclusion with uniform elastic modulus, embedded in an infinite matrix of uniform elastic modulus, using the superposition principle of linear elasticity and using the Green’s function. To obtain this result Eshelby first performed a thought experiment on homogenous infinite elastic body, illustrated in figure 3.2.1.

![Figure 3.2.1: Schematic representation of Eshelby’s problem](image)

The Eshelby’s thought experiment is defined by the following set of imaginary cutting, straining and welding operations:
3.2 Review of MFH techniques

(1) Isolate the ellipsoidal volume from the matrix, the new state of matrix is defined by zero strain and zero stress. The inclusion is subjected to the so-called stress free eigenstrain ($\varepsilon^*$), which is defined as the strain that the inclusion would undergo in the absence of the matrix, thus inclusion’s shape will change.

(2) Apply surface traction to the inclusion surface in order to make the inclusion return to its original shape. An elastic strain is used to cancel the free eigenstrain ($\varepsilon^{el} = -\varepsilon^*$). Then a stress will be equal to $(-\varepsilon^{el} : \varepsilon^*)$, where $\varepsilon^{el}$ is the Hooke’s elastic operator.

(3) Put the inclusion back to the matrix, the applied surface forces on the inclusion’s surface become a layer of body force spread over that surface, in the words of Eshelby.

(4) Now let the body forces relax, i.e remove the traction by applying an opposite body force. The body is now free of external force but in a state of self-stress, due to the inclusion transformation.

Considering the state of the stage (2), using the superposition principle of linear elasticity and using the Green’s function, Eshelby proved that the strain inside the inclusion is related to ($\varepsilon^*$), via a fourth-order tensor known as the Eshelby tensor $\mathcal{E}$:

$$\varepsilon^l = \mathcal{E} : \varepsilon^*$$  \hspace{1cm} (3.2.8)

In the case of ellipsoidal inclusion, it is proved that the stress, strain and displacement inside the inclusion is uniform and $\mathcal{E}$ is a uniform tensor expressed only as a function of the material stiffness tensor and the shape of the inclusion. If the material is isotropic and the ellipsoid of revolution (a spheroid) then $\mathcal{E}$ only depends on the Poisson’s ratio and the ellipsoid’s aspect ratio.

The Eshelby result was used to solve the problem of an isolated inclusion embedded in an infinite matrix, but in this case a uniform strain $\varepsilon^\infty$ is imposed far from the inclusion, on the matrix material boundary. Using the superposition principle of linear elasticity, it could be proved that the strain within the inclusion is related to the imposed strain $\varepsilon^\infty$ as follows:

$$\varepsilon^l = \mathcal{K}_{Eshelby}^e : \varepsilon^\infty$$ \hspace{1cm} (3.2.9)

where $\mathcal{K}_{Eshelby}^e$ is the concentration tensor based on Eshelby’s results and defined by:

$$\mathcal{K}_{Eshelby}^e (\mathbf{T}, \mathcal{C}_{Matrix}, \mathcal{C}_{Inclusion}) = [\mathbf{I} + \mathbf{E} : (\mathcal{C}_{Matrix}^{-1} : \mathcal{C}_{Inclusion} - \mathbf{I})]^{-1}$$ \hspace{1cm} (3.2.10)

The argument $\mathbf{T}$ stands for inclusion’s shape and orientation.

Remark. The Eshelby tensor presents only minor and not major symmetries. Then the so-called Hill tensor $\mathcal{P} = \mathcal{E} : \mathcal{C}_{Matrix}^{-1}$, which has both the minor and major symmetries, is usually employed, as proposed by Hill (1965b).
### 3.2 Review of MFH techniques

**Dilute inclusion model** In this model, each inclusion is considered to be isolated in an infinite medium having the properties of the matrix. The interaction between inclusions is neglected. Then the solution of a single ellipsoidal particle in an unbounded domain given by Eshelby can be used and the concentration tensor is $\mathbf{h}^c = \mathbf{h}_{Eshelby}^c$. The dilute inclusion model is usually used only for composite materials containing a very low volume fraction of inclusions.

**Mori-Tanaka (M-T) scheme** The M-T model (Mori and Tanaka, 1973) supposes that all inclusions have the same shape and are aligned. For this model, and according to the interpretation of Benveniste (1987) each inclusion is considered as isolated in an infinite medium having the matrix properties, and subjected on its boundary to the average strain in the matrix phase of the actual multiple inclusions RVE. The strain concentration is found to be identical to that of the isolated inclusion problem.

$$\mathbb{B}_{M-T} (\mathbf{T}, C_{\omega_0}, C_{\omega_1}) = [\mathbb{I} + \mathcal{E} : (C_{\omega_0}^{-1} : C_{\omega_1} - \mathbb{I})]^{-1}$$  \hspace{1cm} (3.2.11)

Usually, the model of M-T is used for moderate concentrations of inclusions (25-30%). For more important concentrations, Lielens et al. (1998) proposed an extension based on a nonlinear interpolation between the original M-T model and another one with reverse material properties.

**Self-consistent (S-C) scheme** The S-C scheme is also employing Eshelby’s result. It was originally proposed for the prediction of the effective behavior of polycrystals (e.g. Hershey, 1954; Kröner, 1960; Hill, 1965c). Each grain is considered as an ellipsoidal inclusion embedded within a fictitious homogenous matrix having the (yet unknown) stiffness of the actual RVE, and the stress concentration tensor $\mathbf{h}^c$ is

$$\mathbf{h}^c = \mathbf{h}_{Eshelby}^c (\mathbf{T}, \mathbf{C}, C_{\omega_1})$$  \hspace{1cm} (3.2.12)

The stiffness tensor ($\mathbf{C}$) of the matrix surrounding each inclusion is that of the whole RVE and is obtained based on an iterative loop over all grains.

#### 3.2.1.2 MFH of linear thermo-elastic composites

For a two phase linear thermo-elastic composite, the local constitutive equations of each phase ($i \in \{0, 1\}$) can be written as:

$$\sigma_{\omega_i} (x) = C_{\omega_i} : \epsilon_{\omega_i} (x) + \left( -C_{\omega_i}^{\text{el}} : \alpha_{\omega_i} \Delta T (x) \right), \quad i \in \{0, 1\}$$  \hspace{1cm} (3.2.13)

where $C_{\omega_i}$ and $\alpha_{\omega_i}$ are respectively elastic stiffness tensor and second order tensor of thermal expansion for each phase. $\Delta T$ is a uniform temperature variation within all the composite. According to the method proposed by Lielens et al. (1998), the average strain within the inclusion is found to be related to the macro strain $\langle \epsilon \rangle_{\omega_i}$ by the following expression:

$$\langle \epsilon \rangle_{\omega_i} = \mathbf{h}^c : \langle \epsilon \rangle_{\omega_i} + \alpha^c$$  \hspace{1cm} (3.2.14)

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with the strain $a^\varepsilon$ is given by:
\[
a^\varepsilon = (h^\varepsilon - \mathbb{I}) : (C_{\omega_1} - C_{\omega_0})^{-1} : (\beta_{\omega_1} - \beta_{\omega_0})
\] (3.2.15)

The overall average stress is expressed as:
\[
\langle \sigma \rangle_{\omega_1} = C_\omega : (\varepsilon)_{\omega} + \beta_{\omega}
\] (3.2.16)

with the overall stiffness tensor $C_\omega$ is identical to the one in the case of isothermal composite (cf. equation 3.2.5) and the polarization part $\beta_{\omega}$ is defined as:
\[
\beta_{\omega} = v_1 \beta_{\omega_1} + (1 - v_1) \beta_{\omega_0} + v_1 (C_{\omega_0} - C_{\omega_1}) : a^\varepsilon
\] (3.2.17)

3.2.1.3 MFH of linear viscoelastic composites

Each phase $(i \in \{0, 1\})$ of a two phase linear viscoelastic composite, obeys a history-dependent material model which can be defined using the following integral form:
\[
\sigma_{\omega_i}(t) = \int_{-\infty}^{t} C_{\omega_i}^{\varepsilon \varepsilon} (t - \tau) : \frac{\partial \varepsilon_{\omega_i}(\tau)}{\partial \tau} d\tau
\] (3.2.18)

where $\sigma_{\omega_i}, \varepsilon_{\omega_i}$ and $C_{\omega_i}^{\varepsilon \varepsilon}$ are respectively the stress, the strain and the fourth order relaxation tensor. In order to predict the overall behavior of the composite, the Laplace-Carson transformation is employed to obtain an elastic-like form in Laplace-Carson space. The transform function of Laplace-Carson of a given function $f(t)$ is defined by:
\[
f^*(s) = s \int_{0}^{+\infty} f(t) \exp(-st) dt
\] (3.2.19)

The application of the above transform function to the equation 3.2.18, gives the following relation:
\[
\sigma_{\omega_i}^*(s) = C_{\omega_i}^{\varepsilon \varepsilon \star} (s) : \varepsilon_{\omega_i}^* (s)
\] (3.2.20)

The obtained relation (3.2.20) allows to apply the homogenization schemes of linear elastic composites. Once the MFH is performed in the Laplace-Carson space, an inverse transformation, that is usually performed numerically, is employed in order to obtain the results of the homogenization in the time domain. Further details could be found for example in the work of Friebel et al. (2006).

3.2.2 MFH techniques extensions for nonlinear composites

Extending the homogenization techniques from linear to nonlinear behavior is usually based on defining a linear comparison composite (LCC), which is an auxiliary problem (Hill (1965a)) that allows the use of classical results of linear behaviors. Two classes of methods are generally employed in this purpose: methods based on a linearization of the constitutive behavior of each phase and variational methods.
3.2 Review of MFH techniques

3.2.2.1 Methods based on direct linearization of local nonlinear constitutive behaviors

The so-called direct methods are based on a linearization of the constitutive equations of each phase, and considering a linear comparison composite (LCC) having a uniform fictitious instantaneous stiffness operator for each phase. This operator is assumed to be uniform contrary to the instantaneous stiffness operator (tangent or secant) given by the nonlinear constitutive equations, which is not uniform even if the material phase is homogenous.

Many cases of E-P and E-VP composites were investigated in the literature. Recently the behavior of VE-VP composites was investigated by Miled et al. (2013). The problem of composites with non linear behaviors, such as E-P behaviors was addressed very early by several authors such as Kröner (1961); Hill (1965a), who employed the S-C scheme. Kröner (1961) assumed that the plastic deformation can be treated as the eigenstrain of the isolated inclusion in the sense of Eshelby. Based on the mathematical structure of the nonlinear constitutive equations of the phase’s behavior, several linearization methods are commonly used. Hill (1965b) used the tangent stiffness in an incremental way, with the SC scheme. This is considered to be the first version of the incremental linearization method. Later, various linearization methods were proposed such as secant method, affine methods and more recently incremental affine method. The latter methods are generally qualified to be first order MFH methods, higher order MFH methods schemes also exist such as those based on statistical second order moments which help to take into account the field fluctuations inside the phases with respect to the mean (volume average values). In this section a brief presentation of several first order linearization methods, and their applications to non-linear composites is given.

The linearization of the local nonlinear constitutive relations in each phase usually gives a relation with the following form:

\[ \sigma_{\omega_i}(x, t) \approx \mathbf{C}^L_{\omega_i}(t) : \varepsilon_{\omega_i}(x, t) + \tau^L_{\omega_i}(t) \]  \hspace{1cm} (3.2.21)

where \( \mathbf{C}^L_{\omega_i} \) is a uniform comparison elastic stiffness and \( \tau^L_{\omega_i} \) a uniform possible polarization stress, corresponding to the Linear comparison composite (LCC). The LCC should be representative of the real nonlinear composite response for a given time step (cf. figure 3.2.2).

**Secant methods** The secant method was initially also developed for elasto-plastic composites. It is based on the second operator \( \mathbf{C}^{sec} \) (cf. illustration 3.2.3). The stress-strain relation is approximated as follows:

\[ \sigma = \mathbf{C}^{sec} : \varepsilon \] \hspace{1cm} (3.2.22)

where the secant operator is isotropic for locally isotropic materials and is defined as a function of the so-called equivalent strain \( \varepsilon^{sec}_{eq} \) as:

\[ \mathbf{C}^{sec} = 3\kappa^{sec} I^{vol} + 2\mu^{sec} (\varepsilon^{sec}_{eq}) I^{dev} \] \hspace{1cm} (3.2.23)

The approximation 3.2.22 allows to employ the homogenization techniques for thermo-elastic composites, without modification. The equivalent strain is computed by two methods:
3.2 Review of MFH techniques

- By a first order method, which is the classical method of (Berveiller and Zaoui, 1978; Tandon and Weng, 1988), \( \varepsilon_{eq}^{sec} \) is equal to the deviatoric part of the average of the strain tensor in each phase.

\[
\varepsilon_{eq}^{sec} = \left( \frac{2}{3} \langle \varepsilon \rangle^{dev} : \langle \varepsilon \rangle^{dev} \right)^{1/2}
\]  

(3.2.24)

- A modified secant method, known as the second order secant method was proposed in several works (e.g. Casañeda, 1991; Suquet, 1995). \( \varepsilon_{eq}^{sec} \) is defined as:

\[
\varepsilon_{eq}^{sec} = \left( \frac{2}{3} I^{dev} : \langle \varepsilon \otimes \varepsilon \rangle \right)^{1/2}
\]

(3.2.25)

The second order formulation showed better predictions compared to the classical formulation, especially for EP composites. However, in both formulations, the secant method is limited to monotonic and proportional loadings. The case of cyclic loadings cannot be handled by this linearization method. Then it cannot be used in this present work, since the focus is on cyclic loading.

![Diagram](image)

Figure 3.2.2: (Left): The real RVE of the composite using local constitutive equations, (Middle): The LCC, (Right): The equivalent homogeneous material

**Incremental approaches**  As mentioned above the incremental formulation was proposed by Hill (1965a) in order to model the behavior of polycrystals with rate-independent elasto-plastic phases. Incremental approaches are based on a rate formulation of the local problem:

\[
\dot{\sigma} = C^{tan} : \dot{\varepsilon}
\]

(3.2.26)

where \( C^{tan} \) is a tangent operator. For the case of E-P material behavior \( C^{tan} \) is equal to the continuum E-P tangent operator \( C_{el}^{tan} \). An approximation of the stress increment, after a time discretization employing another tangent operator \( C^{alg} \) called algorithmic:

\[
\Delta \sigma \approx C^{alg} : \Delta \varepsilon
\]

(3.2.27)

For each time increment, one of the schemes used for linear composites can be employed. It was employed for various two-phase E-P composites together with a M-T scheme, by several authors (Doghri and Ouaar, 2003; Doghri and Friebel, 2005; Chaboche et al., 2005; Pierard et al., 2007). They employed
the so-called isotropic operator, which enabled to obtain better predictions compared to the original formulation.

The incremental linearization method was also used for nonlinear composites with rate dependent behaviors, such the E-VP composites. Although no continuum tangent operator could be found for E-VP, an algorithmic tangent does exist (e.g. Ju, 1990; Doghri, 2000) and it was used in an incremental way, similar to the E-P case. However, based on the constitutive equation of E-VP, the so-called affine methods are more suitable for rate-dependent phase behavior, since it employs a polarization tensor modeling the effect of loading rate.

Affine methods The affine method was originally developed by several authors (Molinari et al., 1987; Masson and Zaoui, 1999; Masson et al., 2000). It is based on a linearized stress-strain relation involving a polarization stress (τ):

\[ \sigma = C^{tan} : \varepsilon + \tau \] (3.2.28)

Their proposal leads to a thermo-elastic relations in the Laplace-Carson (L-C) domain. This approach was enhanced for two-phase E-VP composites with internal variables by (Pierard and Doghri, 2006a,b).

Figure 3.2.3: Illustration of different linearization methods of nonlinear stress-strain relation, using different operators at given time (t): Elastic operator \( C^{el} \), secant operator \( C^{sec} \) and tangent operator \( C^{tan} \).
3.2 Review of MFH techniques

**Incrementally affine methods** Doghri et al. (2010a) proposed an "incrementally affine" procedure which extends the incremental procedure to E-VP (cf figure 3.2.4). It is based on an interplay between constitutive equations and numerical algorithms. The evolution equations for inelastic strain and internal variables at the beginning of each time interval are linearized around the ending time of the same interval. The linearized equations are then numerically integrated using a fully implicit backward Euler scheme. The obtained algebraic equations lead to an incrementally affine stress–strain relation which involves the algorithmic tangent operator and an affine strain increment $\Delta \varepsilon^{aff}$:

$$\Delta \sigma \approx C^{alg} : (\Delta \varepsilon - \Delta \varepsilon^{aff})$$

(3.2.29)

The proposal leads to thermoelastic-like relations directly in the time domain with stiffness $C^{alg}$ and polarization stress $-C^{alg} : \Delta \varepsilon^{aff}$, and not in the Laplace–Carson (L–C) one. More recently, Miled et al. (2013) extended the work of Doghri et al. (2010a) to VE-VP composites.

![Figure 3.2.4: Illustration of the incrementally affine linearization method in the case of uniaxial tension. Form Doghri et al. (2010b)](image)

3.2.2.2 Variational methods

In the definition of the LCC, methods based on a so-called variational representation are also used. Hereafter a brief reminder of the variational representation in the case that the local constitutive behavior in each phase $\omega_i$ are derived
from a single convex potential $W_{\omega_i}$. The stress-strain relation may be defined by:

$$\sigma_{\omega_i} = \frac{\partial W_{\omega_i}}{\partial \varepsilon_{\omega_i}} \quad (3.2.30)$$

The minimum energy principle should be satisfied with the strain field ($\varepsilon$) within the composite material. Thus the average strain energy $\langle W \rangle_{\omega}$ is defined by the following minimization problem:

$$\langle W \rangle_{\omega} = \min_{\varepsilon \in \mathcal{K} (\varepsilon)} \left( v_1 \langle W (\varepsilon) \rangle_{\omega_1} + (1 - v_1) \langle W (\varepsilon) \rangle_{\omega_0} \right) \quad (3.2.31)$$

where $\mathcal{K} (\varepsilon)$ is the set of kinematically admissible strain fields. The relation between the macro-stress and macro-strain is derived from $\langle W \rangle_{\omega}$ as:

$$\langle \sigma \rangle_{\omega} = \frac{\partial \langle W \rangle_{\omega}}{\partial \langle \varepsilon \rangle_{\omega}} \quad (3.2.32)$$

The variational representation allows to obtain a more complex definition of LCC compared to the direct linearization of constitutive behaviors. Examples of those works are the work of Ponte Castañeda et al. (e.g. Castañeda, 1991; Castañeda, 1992; Castañeda, 1996) on heterogeneous hyper-elastic materials and the works of Brassart et al. on E-P composites (Brassart et al., 2011) and on E-VP composites (Brassart et al., 2012).

### 3.2.3 MFH techniques extensions for multiphase and misaligned inclusions reinforced composites

Among the most challenging types of composites, from modeling point of view and which several multiscale homogenization techniques have been trying to model are composites reinforced with discontinuous and misaligned fibers, such as the SFRTPs studied in this work. The first element to be solved when dealing with this problem is the fibers orientations: how to obtain a realistic modeling of them, and how to measure their effect on the material behavior. Several attempts to model the orientation of the short fibers or inclusions, are mainly based on the concept of orientation tensors (e.g. Advani and Tucker III, 1987) which are obtained either experimentally or numerically by taking into account the material manufacturing process. Orientation tensors are expressed either as a second order or as a fourth order tensor, and they are functions of an Orientation Distribution Function (ODF) defining the probability of having inclusions oriented near a given direction. New numerical tools simulating the manufacturing process such as the injection molding process allow to estimate the orientation tensor. However, in several homogenization techniques of the material behavior, a reconstruction of the ODF is needed. The length distribution (LDF) function is also needed in order to have an accurate representation of RVEs.

In order to use MFH techniques for the case of composites with misaligned and non identical inclusions, and take into account the information given by ODF and LDF, two methods are being employed based on an extension of the existing techniques. The first one is the so-called direct method or the single
3.2 Review of MFH techniques

The direct method consists in generalizing the same procedure for two phase composite (cf. section 3.2.1.1) to multiphase composites. The overall stiffness is expressed as follows:

$$C_\omega = C_{\omega_0} + \sum_{i=1}^{M} v_i (C_{\omega_i} - C_{\omega_0}) : A_{\omega_i} \quad (3.2.33)$$

where $A_{\omega_i}$ represent the concentration tensors and $C_{\omega_i}$, $v_i$ are the stiffness and the volume fraction of each phase among the $M$ phases. More details about this generalization of classical methods applied to two phase composites may be found in Benveniste et al. (1991); Benveniste (1987). The most famous example of one step method, is indeed the Mori and Tanaka (M-T) model which was formulated for a number (M) of inclusions without assuming that they are identical or aligned. However the formulation when applied to multiphase composites may give physically inadmissible solutions. According to Benveniste et al. (1991) the Mori-Tanaka and the self-consistent models return diagonally symmetric results only for two-phase systems and for those multiphase systems in which the dispersed phases are aligned and of similar shape. Thus, another method is usually used instead of direct method. The so-called pseudo-grain decomposition method, also-called two step method is based on the concept of pseudo-grains (PGs). The PGs are micro-domains grouped numerically into a single domain (cf. figure 3.2.5) viewed as a two-phase classical composite which contains matrix material and all inclusions which have the same material, aspect ratio and orientation. The relative weight of each PG inside the RVE is derived from the ODF and the LDF. Usually the Mori-Tanaka scheme is used for the homogenization of each PG, and Voigt scheme in the second homogenization in order to obtain the overall behavior. Examples of works employing this approach are Lielens et al. (1998); Doghri and Tinel (2005); Kammoun et al. (2011b, 2015). In this present work, the PG decomposition is employed since it gives always physically admissible results.

Figure 3.2.5: Schematic representation of the pseudo-grain decomposition based homogenization procedure
3.3 MFH of a two phase VEVPD composite

In this section, the incrementally affine linearization method presented in section 3.2.2.1 is employed in order to predict the homogenized behavior of a VEVPD composite. Several cases can be treated with the VEVPD model, by setting appropriate values of some material parameters, thus it allows to have a general framework applicable for several types of composites.

For each phase \((i)\) of the composite the behavior is assumed to be VEVPD. The subscript \(\omega_l\) is omitted for the sake of clarity. As detailed in Appendix B, for VEVPD model the increment of the effective stress is linked to the increment of strain in each time step by the following expression:

\[
\Delta \tilde{\sigma} = \tilde{\sigma} (t_{n+1}) - \tilde{\sigma} (t_{n}) = \tilde{\mathcal{C}}^{\text{eff}} (\Delta \tilde{\epsilon}) : (\Delta \tilde{\epsilon} - \Delta \tilde{\epsilon}^{\text{vp}}) + a(t_{n}) \tag{3.3.1}
\]

where

\[
a(t_{n}) = - \sum_{i=1}^{L} \left[ 1 - \exp \left( - \frac{\Delta t}{g_i} \right) \right] \tilde{s}_i(t_{n}) - \sum_{j=1}^{J} \left[ 1 - \exp \left( - \frac{\Delta t}{k_j} \right) \right] \tilde{H}_j(t_{n}) I \tag{3.3.2}
\]

The expression of the viscoplastic strain increment is found using the procedure proposed by Doghri et al. (2010a) for EVP composites. The following notation are used hereafter, for the evolution of the VP strain and the scalar or tensor the scalar and/or tensor internal variables \((V)\) and their derivatives:

\[
\dot{\epsilon}^{\text{vp}}(t) = \dot{\epsilon}(\sigma (t), V (t)) ; \dot{\epsilon}, \sigma = \frac{\partial \dot{\epsilon}}{\partial \sigma} ; \dot{\epsilon}, V = \frac{\partial \dot{\epsilon}}{\partial V} \]

\[
\dot{V} (t) = \dot{V} (\sigma (t), V (t)) ; \dot{V}, \sigma = \frac{\partial \dot{V}}{\partial \sigma} ; \dot{V}, V = \frac{\partial \dot{V}}{\partial V} \]

The increment of viscoplastic deformation is then expressed as :

\[
\Delta \epsilon^{af} = \left[ \dot{\epsilon}^{\text{vp}} (t_{n}) + \dot{\epsilon}, V (t_{n+1}) \bullet \ldots \right]^{-1} \bullet \dot{V} (t_{n}) + \{\ldots \} : \Delta \sigma \Delta t \tag{3.3.3}
\]

where the bullet symbol “\(\bullet\)” designates a sum of inner products and \(I\) designates an identity tensor of the same rank to \(V\), such that \((V \bullet I = I \bullet V = V)\).

The expressions \([\ldots]\) and \(\{\ldots\}\) are given by:

\[
[\ldots] = \frac{1}{\Delta t} I - \dot{V} (V (t_{n+1})) \tag{3.3.4}
\]

\[
\{\ldots\} = \dot{\epsilon}, \sigma (t_{n+1}) + \dot{\epsilon}, V (t_{n+1}) \bullet \ldots^{-1} \bullet \dot{V}, \sigma (t_{n+1}) \tag{3.3.5}
\]

After substituting the expression of \((\Delta \epsilon^{\text{vp}})\) in equation 3.3.1, the increment of the effective stress can be written as:

\[
\Delta \tilde{\sigma} = \tilde{\mathcal{C}}^{\text{alg}} (t_{n+1}) : (\Delta \tilde{\epsilon} - \Delta \epsilon^{af}) \tag{3.3.6}
\]

where the \(\tilde{\mathcal{C}}^{\text{alg}}\) is the effective algorithmic tangent operator at time \(t_{n+1}\) and \(\Delta \epsilon^{af}\) is an affine strain increment.
3.3 MFH of a two phase VEPD composite

\[ \tilde{C}^{alg}(t_{n+1}) = \left( \tilde{C}^{ve} \right)^{-1} \]  (3.3.7)

\[ + \Delta t \left\{ \bar{\epsilon}_\sigma(t_{n+1}) + \bar{\epsilon}_{\dot{V}}(t_{n+1}) \cdot \left[ \frac{1}{\Delta t} I - \tilde{\dot{V}}_V(t_{n+1}) \right]^{-1} \cdot \tilde{\dot{V}}_\sigma(t_{n+1}) \right\} \]^{-1}

with \( \dot{V} = (r, X_{ij}, D) \). The affine strain increment (\( \Delta \epsilon^{af} \)) is expressed by:

\[ \Delta \epsilon^{af} = \Delta \epsilon^{af}_{ve} + \Delta \epsilon^{af}_{vp} \]  (3.3.8)

here \( \Delta \epsilon^{af}_{vp} \) is given by the following expression:

\[ \Delta \epsilon^{af}_{vp} = \bar{\epsilon}^{vp}(t_n) + \bar{\epsilon}_{\dot{V}}(t_{n+1}) \cdot \left[ \frac{1}{\Delta t} I - \tilde{\dot{V}}_V(t_{n+1}) \right]^{-1} \cdot \tilde{\dot{V}}(t_n) \Delta t \]  (3.3.9)

And the \( \Delta \epsilon^{af}_{ve} \) is expressed as:

\[ \Delta \epsilon^{af}_{ve} = - \left( \tilde{C}^{ve} \right)^{-1} : \bar{\epsilon}(t_n) \]  (3.3.10)

By replacing the expression of \( \bar{\epsilon}(t_n) \) and \( \tilde{C}^{ve} \) in the expression of \( \Delta \epsilon^{af}_{ve} \), we find:

\[ \Delta \epsilon^{af}_{ve} = \frac{1}{2G} \sum_i \left[ 1 - \exp \left( -\frac{\Delta t}{g_i} \right) \right] \tilde{\sigma}_i(t_n) \]

\[ + \frac{1}{2K} \sum_j \left[ 1 - \exp \left( -\frac{\Delta t}{k_j} \right) \right] \tilde{\sigma}_H_j(t_n) I \]  (3.3.11)

On the other hand, using the definition of the effective stress:

\[ \Delta \sigma = (1-D)\Delta \tilde{\sigma} - \tilde{\sigma} \Delta D \]  (3.3.12)

It is finally found that:

\[ \Delta \sigma = (1-D)\tilde{C}^{alg} : \Delta \epsilon + \Delta \tau \]  (3.3.13)

with

\[ \Delta \tau = - (1-D)\tilde{C}^{alg} : \Delta \epsilon^{af} - \tilde{\sigma} \Delta D \]  (3.3.14)

The expression of \( \Delta \tau \) is a function of \( \Delta \epsilon^{af}_{vp} \), which is a too complex function which is not obvious to be found. Thus, similar to the proposal of (Doghri et al., 2010a) for EVP as an alternative, \( \Delta \tau \) will be computed using equation (3.3.13) since the other quantities are all given by the VEPD constitutive material behavior.

Doghri et al. (2010a) and Miled et al. (2013) use an extracted isotropic tangent operator in order to replace the algorithmic tangent operator, because it is known that using an anisotropic tangent, such as the tangent operator in the computation of the Eshelby, Hill tensors, may lead to too stiff predictions as illustrated by Pierard and Doghri 2006a,b for EP or EVP composites, using affine or incremental methods. Several methods are used in order to obtain an isotropic tangent operator, such as general isotropic extraction or more sophisticated isotropic extraction methods, for example the spectral decomposition.
method Castañeda (1996). In this work the general isotropic extraction will be used, but applied to effective algorithmic tangent operator. The main idea is to find two scalars: tangent bulk $\kappa_t$ and shear moduli $\mu_t$, which allow to define the isotropic tangent operator $\tilde{\mathbf{C}}^{iso}$ as:

\[
\tilde{\mathbf{C}}^{iso} = 3\kappa_t I^{vol} + 2\mu_t I^{dev}
\]  

(3.3.15)

Then in equation 3.3.13 $\tilde{\mathbf{C}}^{alg}$ is replaced by $\tilde{\mathbf{C}}^{iso}$ and $\Delta \mathbf{T}$ is computed based on the new expression. For the sake of clarity, the $(1 - D) \tilde{\mathbf{C}}^{iso}$ is replaced by $\mathbf{C}^{tan}$. An illustration of the proposed incrementally affine linearization method is given in the figure 3.3.1.

Figure 3.3.1: Illustration of the proposed incrementally affine linearization method used for VEVPD model in the case of uniaxial tension.

The behavior of the homogenized VEVPD composite material is obtained using mean field homogenization (MFH) techniques. Hereafter, the details of the method development are given, based on an analogy with the thermoelastic composites (see section 3.2.1.2) and using the incrementally affine form already presented. For the VEVPD model, the expression of the stress increment is form-similar to the incrementally affine form found for the matrix and the inclusion. Using the following analogy allows to use the results of MFH for the linear thermo-elastic composites $i \in \{0, 1\}$:

\[
\begin{align*}
\sigma_{\omega_i} & \rightarrow (\Delta \sigma)_{\omega_i} \\
\epsilon_{\omega_i} & \rightarrow (\Delta \epsilon)_{\omega_i} \\
\beta_{\omega_i} & \rightarrow \Delta \mathbf{T}_{\omega_i}
\end{align*}
\]

Using this analogy, the expression of the average of stress increment is found to be:
3.3 MFH of a two phase VEVPD composite

\[
\langle \Delta \sigma \rangle_\omega = C_\omega : \langle \Delta \epsilon \rangle_\omega + v_1 \tau_{\omega_1} + v_0 \tau_{\omega_0} + v_1 (C^{\tan}_{\omega_1} - C^{\tan}_{\omega_0}) : (B^e - I) : (C^{\tan}_{\omega_1} - C^{\tan}_{\omega_0})^{-1} : (\Delta \tau_{\omega_1} - \Delta \tau_{\omega_0}) \tag{3.3.16}
\]

The diagram given in figure 3.3.2 illustrates the numerical algorithm. The aim is to find the strain within the inclusions which satisfy the following equation, obtained also by analogy with the equation 3.2.14 for thermo-elastic composites, as:

\[
\langle \epsilon \rangle_\omega = A^e : \Delta \tilde{\epsilon} + (A^e - I) : (C^{\tan}_{\omega_1} - C^{\tan}_{\omega_0})^{-1} : (\Delta \tau_{\omega_1} - \Delta \tau_{\omega_0}) \tag{3.3.17}
\]

Figure 3.3.2: Algorithm of the homogenization model for VEVPD composites
3.4 Numerical simulations

In this section, some numerical simulations are performed using the proposed MFH method for two phase VEVPD composites. The case of PA66 matrix assumed to obey VEVPD behavior, reinforced with identical and aligned glass fibers assumed to be elastic is treated. In the next chapter, the case a VE matrix with VEVPD inclusions is also treated with the proposed MFH model, in order to solve the problem of fatigue of TPs.

Glass fibers have a Young’s models of $E_f = 70$ GPa. However, in order to model in a single way the effect of a weakened interface and partial debonding, we consider that the fibers are perfectly bonded to the matrix, but have a reduced Young’s modulus $E_f = 30$ GPa. For the PA66 matrix, the experimental data provided by our DURAFIP partners are used to identify the material parameters. The VE parameters are identified using available DMA test, for temperature $T=23$ °C. The values of $E'$ and $E''$ are presented in figure 3.4.1 as function of the frequency. The identified VE elastic parameters are listed in table 3.1.

![Dynamic moduli (E' and E'')]({})

Figure 3.4.1: Experimental (symbol) and analytical (lines) results of storage and loss moduli for PA66 RH50 at $T=23$°C

Tensile tests at different strain rates were conducted by our DURAFIP project partners on unreinforced PA66. Here the focus will be on the small strain deformation. As it could be seen from the experimental data (cf. figure 3.4.2), the material is too sensitive to the strain rate change. The damage is not important according to the stress strain curves but small softening does exist, evidenced by a small drop of the true tensile stress. It is assumed that the PA66 matrix obeys to J2 yielding law, with an isotropic hardening defined by a power law: $R(p) = k.p^n$. Here, $p$ is the accumulated equivalent plastic strain. $k$ and $n$ are material parameters. VP and damage parameters are listed in table 3.2.
3.4 Numerical simulations

![Stress strain curves](image)

Figure 3.4.2: Stress strain curves for PA66 RH50 at T=23°C under different strain rates using a power law isotropic hardening. Lines stand for numerical simulations obtained by VEPVD model and symbols stand for experimental results.

Hereafter the proposed MFH model is employed to simulate the behavior of SGFRPA66 under monotonic tensile loadings. The capabilities of the model to capture the main composite material sensitivities is evaluated by comparison with experimental trends of the SFRTPs in general, as detailed in section 1.2.1 and by comparison with experimental results on PA66 reinforced by short glass fibers, also provided by our DURAFIP project partners. The glass fibers orientation is taken into account by the PGs decomposition method. As shown in the introduction chapter, the material presents a very complex microstructure (cf. figure 1.2.3). For our study as in Kammoun et al. (2011b, 2015), the average orientation tensor over the thickness in the mid-section of dumbbell is used. The weights of pseudo-grains representing different fiber orientations relative to the MFD presented in figure 3.4.3, are used.

The following results are only qualitative, since in order to obtain realistic predictions, the following elements should be taken into account:

- Consider the important role of the interface between the fibers and the matrix in terms of progressive failure. Indeed, at given states of strains and stress the interface is no-longer able to transfer the loading between the matrix and the fibers, which should have important consequences on the macroscopic behavior.

- The damage evolution within the matrix is expected to be different compared to the unreinforced TPs, due to the presence of the fibers.

The former considerations are taken into account by Kammoun et al. (2011b, 2015) by different approaches at the level of each pseudo-grain (cf. section 5.1.3 for an overview about those two models).
3.4 Numerical simulations

<table>
<thead>
<tr>
<th>Poisson’s ratio: $\nu = 0.35$</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_0 = 2500$ MPa</td>
<td></td>
</tr>
<tr>
<td>$E_i$ (MPa)</td>
<td>$\tau_i$ (s)</td>
</tr>
<tr>
<td>422</td>
<td>0.0045</td>
</tr>
<tr>
<td>316</td>
<td>0.055</td>
</tr>
<tr>
<td>250</td>
<td>0.75</td>
</tr>
<tr>
<td>250</td>
<td>2.8333</td>
</tr>
</tbody>
</table>

Table 3.1: Table of VE parameters for PA66 RH50 at $T=23^\circ$ C

Isotropic hardening: $R(p) = k.p^n$ $k = 16.5\sigma_y$ $n = 0.50$

Viscoplastic function: $g_v = \frac{\sigma_Y}{\eta} \left( \frac{f}{\sigma_Y} \right)^m$ $\eta = 417$ MPa.s $m = 6$

Damage parameters: $\dot{D} = \left( \frac{Y}{S} \right)^p$ $S = 0.35$ MPa $s = 0.65$

Table 3.2: VP and damage parameters for PA66 RH50 at $T=23^\circ$ C, $\sigma_y$ is the yield stress.

Figure 3.4.3: Weights of 36 pseudo-grains representing different fiber orientations relative to the MFD. Weights are determined for glass fiber (GF) mass fractions: 20%, 30% and 50%. (From Kammoun et al., 2011b)
3.4 Numerical simulations

3.4.1 Effect of the fiber orientation and strain rates

The available experimental results are obtained at different strain rates and different orientations w.r.t MFD. The assumption of aligned fibers and the PG decomposition method are used in the following simulations. The experimental orientations are $0^\circ$, $45^\circ$ and $90^\circ$. Figures 3.4.4-(a) and 3.4.4-(b) present the predictions of the model using the aligned fibers assumption and using the PG decomposition, respectively. The predictions using the PG decomposition are better than those with the aligned fibers assumption. But for the PG method overestimates the stress mainly in the nonlinear part of the behavior.

![Figure 3.4.4: Stress strain curves of PA66 reinforced with 20% of mass fraction of GF, under different strain rates and for different orientations w.r.t. MFD. Lines stand for numerical simulations: (a) using aligned fibers assumption, (b) using the PG decomposition. Symbols stand for experimental results.](image)

The mean-field method are known to overestimate the nonlinear response of short fiber reinforced Polyamide. That’s why modified spectral isotropisation
method was proposed by Selmi et al. (2011), and employed by Kammoun et al. (2011a, 2015)

In order to test the sensitivity of the model to a change of strain rate for a given microstructure, it was used to simulate the behavior of PA66-GF20 under different strain rates, for 45° orientation w.r.t MFD. As shown in figure 3.4.5, the increase of the strain rate leads to increase of the value of the stress, which is consistent with the experimental trend usually observed for SFRTPs.

Hereafter a parametric study using the volume fraction of the fibers and their aspect ratio is presented. The PG decomposition is used since it gives a better representation of the microstructure.

### 3.4.2 Effect of volume fraction of the fibers and the fibers aspect ratio

Figure 3.4.6-(a) depicts the effect of different values of volume fraction of GF on the stress strain curves of SGFRPA66. The model also reproduces the observed experimental trend: when the volume fraction of the fibers increases, the level of stress that is reached by the material is higher.

The effect of aspect ratio is also simulated using the proposed model. Figure 3.4.6-(b) shows that the higher the aspect ratio the higher the value of stress reached by the material.
3.5 Discussion and possible enhancements

The proposed MFH method for two phase VEVPD composites follows a similar approach to the methods proposed for two phase VEVP composites proposed Miled et al. (2013) and for two phase EVP composites by (Doghri et al., 2010a). The method were extended here in order to take into account damage coupling and nonlinear kinematic hardening. Then the major sensitivities of those proposals are necessarily faced when applying the present MFH model such as the sensitivity to change of time increment, as illustrated in figure 3.5.1. For both (Doghri et al., 2010a) and (Miled et al., 2013), the same solution was used to solve the problem which is the use of a so-called regularization of the
### 3.5 Discussion and possible enhancements

Instantaneous stiffness tensor based on analogy to 1D problem proposed by Doghri et al. (2010a). Figure 3.5.2 is from (Miled et al., 2013) showing the insensitivity of the numerical prediction to the number of time increments. For VEVPD composites solving an equivalent 1D problem is a too complex task, however applying the expression of regularized instantaneous stiffness tensor given by (Miled et al., 2013) to the effective algorithmic tangent operator of the VEVPD model may give good results.

![Figure 3.5.1: Stress strain curves of PA66 reinforced with 20% of short GF, for different values time increment. The loading has a strain rate equal to $10^{-4}$ s$^{-1}$ and applied on the orientation $45^\circ$ w.r.t. MFD.](image)

Unlike linear composites, for nonlinear ones such as VEVPD, field fluctuations inside the phases may have an important role on the macroscopic behavior and on the material failure if the behavior is damaged. For instance, the plastic accumulation field in an E-P matrix reinforced with short elastic fibers is not uniform, as shown by a FE computation performed by Doghri et al. (2011), in order to model the SGFRPA66 (cf. figure 3.5.3). The use of statistical second moments MFH techniques as the one proposed for E(V)P composites Doghri et al. (2011) may improve predictions compared to the first order MFH method proposed in this chapter. MFH schemes with statistical second moments help measure the variance and the field fluctuations inside the phases with respect to the mean (volume average values).
3.5 Discussion and possible enhancements

Figure 3.5.2: Tension test of polycarbonate at the strain rate of $10^{-3}s^{-1}$ for a volume fraction of spherical inclusions equal to 15% with different numbers of time steps (200, 1000 and 10000), using a regularized instantaneous stiffness tensor in the MFH method for VEPV composites. (From Miled et al. 2013)

Figure 3.5.3: Contour plot of the accumulated plastic strain in the matrix of a short glass fiber reinforced Polyamide. The applied macroscopic elongation is 5%, either in the direction of the fibers axis (a) or in the transverse direction (b), from Doghri et al. (2011).
3.6 Conclusion

In this chapter, a review about the existing mean-field homogenization methods for linear and nonlinear two phase composites in isothermal and non-isothermal conditions are given. The existing methods for misaligned and multiphase composites are presented briefly. A proposal for homogenization of two-phase VEVPD composites based on the incremental affine linearization method is developed. Some numerical simulations using the MFH model and possible enhancements are presented. The proposed homogenization method for VEVPD composites is used in solving the problem of fatigue of short fiber reinforced and unreinforced thermoplastics as it will be detailed in chapter 4 for TPs and chapter 5 for SFRTPs.
Chapter 4

A two-scale model for the high cycle fatigue of neat thermoplastic polymers

The aim of this chapter is to propose and evaluate a new modeling approach for TPs under fatigue loading. Thermoplastic homogeneous polymers (TPs) especially the so-called rigid such as high-density polyethylene (HDPE) and Ultra-high-molecular-weight polyethylene (UHMWPE) are being used to replace classical metallic materials in numerous industrial products, namely the massive produced ones, for instance 90% of the new piping installations (for gas, water distribution, etc.) are made with HDPE. Consequently, their modeling is becoming more and more interesting, especially for fatigue design purposes. Based on experimental investigations found in the literature (presented in the introductory chapter) a multiscale approach is proposed.

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</tbody>
</table>
4.1 State-of-the-art description

During its lifetime, a part is subjected to a complex fatigue loading history. In order to simplify the analysis, an idealized loading is generally employed, based on methods such as rainflow count originally proposed by Matsuishi and Endo (1968). The considered loading is either uniaxial (generally called single component loading) or multiaxial. It is defined by blocks of loadings with constant mean, maximum and minimum values. Several methods exist to compute the number of cycles to failure under these blocks of loading (as detailed hereafter) and take into account the mean stress effect, such as (Goodman equation, Gerber equation, etc.) in each block. Using a so-called cumulative damage law such as Miner’s rule (Miner et al., 1945), the total number of cycles to failure under the approximation of the real loading is found.

Several authors extended existing approaches for fatigue already used for metals, assumed to be isotropic and homogenous. As already mentioned in the introduction chapter, the material failure is the result of two processes: the initiation of a crack, and its propagation until the final failure. Based on whether crack initiation or propagation process has the major contribution to the material lifetime, two modeling approaches are proposed.

4.1.1 Crack initiation based approaches

4.1.1.1 Failure criteria based approaches

Several approaches based on failure criteria are proposed in the literature, mainly inspired from the existing criteria for metals. The fatigue failure criteria are designed to estimate a limit state representing failure, similarly to those employed under monotonic loadings. The formulation of those criteria is usually based on using invariants of stress or strain tensors.

Failure criteria are different for low cycle fatigue (LCF) and high cycle fatigue (HCF). Usual LCF criteria employ strain such as Manson–Coffin model or are based on energy considerations. However usual HCF criteria use mainly stress based failure criteria. Hereafter, a selection of those criteria is presented.

Stress based failure criteria  The material behavior is generally assumed to be elastic. The basic idea is to separate the stress space into two regions, unsafe and safe. The operation is made using a closed surface containing the origin and bounding the safe region, similar to approaches based on static yield stress employed in the case of monotonic loadings. Their ingredients are the hydrostatic stress and the second invariant of the stress deviator (Papadopoulos et al., 1997). In case of a single stress component usually used for fatigue testing, those quantities are easy to obtain compared to multiaxial loading case. For a general cyclic loading, the stress tensor may be split in a deviatoric and spherical part as:

\[ \sigma = s + \frac{1}{3} \text{tr} (\sigma) I \quad (4.1.1) \]

The hydrostatic stress is a scalar periodic function of time with period \( T \) defined by:
4.1 State-of-the-art description

\[ \sigma_H = \frac{1}{3} \text{tr}(\sigma) \]  

(4.1.2)

The hydrostatic stress amplitude \( \sigma_{H,\alpha} \), the mean value \( \sigma_{H,m} \) and the maximum value \( \sigma_{H,max} \) are defined respectively by:

\[
\sigma_{H,\alpha} = \frac{1}{2} \left\{ \max_{t \in [0,T]} (\sigma_H(t)) - \min_{t \in [0,T]} (\sigma_H(t)) \right\} 
\]  

(4.1.3)

\[
\sigma_{H,m} = \frac{1}{2} \left\{ \max_{t \in [0,T]} (\sigma_H(t)) + \min_{t \in [0,T]} (\sigma_H(t)) \right\} 
\]  

(4.1.4)

\[
\sigma_{H,max} = \sigma_{H,\alpha} + \sigma_{H,m} 
\]  

(4.1.5)

For the deviatoric part, defining the amplitude \( (\sqrt{J_{2,\alpha}}) \) and the mean value \( (\sqrt{J_{2,m}}) \) is a more difficult task compared to the hydrostatic stress. For this purpose, several methods are proposed (e.g. Papadopoulos et al., 1997; Weber et al., 1999; Zouain et al., 2006). The proposal of Papadopoulos et al. (1997) is detailed hereafter. They used the following transformation rules:

\[
S_1 = \frac{\sqrt{3}}{2} s_{xx}; \quad S_2 = \frac{1}{2} (s_{yy} - s_{zz}); \quad S_3 = s_{xy} 
\]  

(4.1.6)

\[
S_4 = s_{xz}; \quad S_5 = s_{yz} 
\]

The above rules allow to map the stress deviator tensor \( s \) onto a vector \( S \) of a five-dimensional Euclidean space denoted \( E_5 \). Then the second invariant may be expressed as:

\[
\sqrt{J_2} = \sqrt{\frac{1}{2} S : S} = \sqrt{S \cdot S} 
\]  

(4.1.7)

According to Papadopoulos et al. (1997), during a periodic loading the tip of the vector \( S \) describes a closed curve \( \phi \) in \( E_5 \). In order to find \( \sqrt{J_{2,\alpha}} \), a minimum five-dimensional hypersphere, assumed to be unique, circumscribed to the curve \( \phi \), need to be constructed. The length of the vector \( S_m \) that points to the center of this hypersphere is equal to \( \sqrt{J_{2,m}} \), and \( \sqrt{J_{2,\alpha}} \) is equal to the radius of this sphere. \( S_m \) is found by solving the following min-max problem:

\[
S_m : \min_{S} \max_{t \in [0,T]} \| S(t) - S' \| 
\]  

(4.1.8)

Then the \( \sqrt{J_{2,\alpha}} \) is defined by:

\[
\sqrt{J_{2,\alpha}} = \max_{t \in [0,T]} \| S(t) - S_m \| 
\]  

(4.1.9)

Several criteria were formulated using the above quantities, among the most used and applied to TPs, one can cite Sines and Crossland criteria, that are detailed hereafter (cf. Papadopoulos et al. (1997) for a selection of the main fatigue criteria used for metals).

- **Sines criterion**

The criterion proposed by Sines (1959) is written as:

\[
\sqrt{J_{2,\alpha}} + \alpha_{Si} \sigma_{H,m} \leq \beta_{Si} 
\]  

(4.1.10)

Where \( \alpha_{Si} \) and \( \beta_{Si} \) are material parameters.
4.1 State-of-the-art description

- Crossland criterion

A similar criterion was formulated by Crossland (1956). The difference is the use of the maximum of hydrostatic stress $\sigma_{H,max}$ instead of $\sigma_H$ (cf. expression 4.1.11).

$$\sqrt{J_2,n} + \alpha_{Cr} \sigma_{H,max} \leq \beta_{Cr}$$  \hspace{1cm} (4.1.11)

Where $\alpha_{Cr}$ and $\beta_{Cr}$ are material parameters.

Several authors employed the existing failure criteria with or without modification in order to predict the S-N curves mainly of testing samples of TPs. An example of those works is the work of Berrehili et al. (2010b, a) on the fatigue of HDPE. They showed that the previous criteria are not able to capture the effect of multiaxial loadings and the sensitivity to the mean stress. In order to capture those effects, they proposed the following criterion which gives a better correlation with their experimental results, defined by the following expression:

$$\sqrt{J_{2,max}} + \alpha J_{2,m} \leq \beta_{Cr} + \frac{A}{(N_f)^c}$$ \hspace{1cm} (4.1.12)

where $\alpha$, $\beta_{Cr}$, $A$, and $c$ are material parameters. $N_f$ is the number of cycles to failure.

For the presented criteria, the material parameters are generally identified based on endurance or fatigue limits of the materials, the latter are still a matter of discussion for polymers and composite-based polymers since it is not always observed in this kind of materials.

Strain based approach  Another kind of criteria are the ones employing the strain in finding a good correlation with the fatigue failure. Usually employed in the case of LCF loading, generally obtained in the case of high level of stress, which will create plastic deformations. Among the most famous criteria based on strain, one can cite the model defined by the so called Manson-Coffin equation (Coffin Jr, 1954; Manson, 1954). It has been originally proposed for predicting the LCF life of metals in uniaxial tests, assumed to obey to an EP behavior. It links the plastic strain ($\varepsilon_p$) to the number of cycles to failure ($N_r$). The criterion is defined by this expression:

$$\varepsilon_p (N_f)^\alpha = C$$ \hspace{1cm} (4.1.13)

where $\alpha$ and $C$ are material parameters.

4.1.1.2 Progressive failure based approaches

More sophisticated constitutive model than the elastic and elasto-plastic models, employed in previous failure criteria, are proposed in order to model the different progressive phenomena which may be responsible of initiation of a crack, such as softening and physical aging. An example of these models is the finite strain formulated elasto-viscoplastic model of Klompen et al. (2005) (see section 2.1 for more details about this model). The model was employed by Janssen et al. (2008a) in order to predict the behavior of several TPs under fatigue loadings.
4.1 State-of-the-art description

The authors assumed similarities in deformation and failure kinetics under creep and cyclic loadings. The model was employed to predict the behavior of polycarbonate (PC) based on an axisymmetric FE model of the specimen with a small imperfection in the middle. The material failure is defined at the moment at which a macroscopic strain reaches a critical value found experimentally (cf. figure 4.1.1).

Figure 4.1.1: Experimental time-to-failure of PC under stress loading (55 MPa) is determined at a macroscopic strain of 20% (From Janssen et al., 2008a).

An analytical 1-D method is also proposed by Janssen et al. (2008b) using a critical value of plastic strain at which softening occurs. The later model is a simplified model using the creep failure data to estimate the failure under fatigue loading, which gives good correlation with experimental results. However it doesn’t take into account a multi-axial fatigue loading.

4.1.2 Crack propagation based approach

Crack propagation is usually modeled using fracture mechanics. Fracture mechanics based approaches are considered to be the most classical approaches. They assume that a material always contains defects, however, they always ignore the initiation stage of the failure. A notched specimen is usually used to study the crack propagation within a material. A well-known model is that of Paris and Erdogan (1963), based on the work of Griffith (1921), was developed initially for metals. It gives the rate of crack propagation per cycle as a function of the variation of the so-called stress intensity factor:
4.1 State-of-the-art description

\[ \frac{da}{dN} = m_0 \Delta K^n \]  

(4.1.14)

where \((\Delta K = K_{\text{max}} - K_{\text{min}})\) is the amplitude of the stress intensity factor, \(a\) is the crack length. \(m_0\) and \(n\) are material constants. The stress intensity factor \(K\) is defined by:

\[ K = \frac{P}{hW} \sqrt{aY} \left( \frac{a}{W} \right) \]

where \(a\) is the crack length, \(P\) the force, \(Y\) the geometry factor, \(h\) and \(W\) are respectively the thickness and the length of the sample. Fracture will happen when the intensity factor reaches a critical value \(K_c\). The Paris–Erdogan equation (PEE) models the region II in the well-known crack propagation diagram (cf. figure 4.1.2, for details about the other regions).

Figure 4.1.2: Different regions of crack propagation. In region I the crack propagation rate decreases rapidly to a limit \(\Delta K_{\text{th}}\). Since below this limit no crack propagation can be detected, the knowledge of \(\Delta K_{\text{th}}\) is of special importance for component design. Region II, describes in the double-logarithmic scale a region of stable crack growth, which is characterized by the Paris–Erdogan Equation (PEE). In region III of the diagram the crack propagation rate increases more quickly up to the limit \(\Delta K_{\text{crit}}\), where the crack in a fatigue experiment becomes unstable during one load cycle.(From Kallrath et al., 1999)

Examples of references applying the Paris–Erdogan equation for both polymers and polymer composites are (Williams, 1977; Kallrath et al., 1999), based on the fundamental assumption that the fatigue lifetime of the material is determined by the duration of the crack propagation phase.
4.1 State-of-the-art description

4.1.3 Summary

In summary, the main existing modeling approaches for TPs fatigue are classified in two categories: Crack initiation based approaches and crack propagation based approaches. As mentioned in the introduction chapter, according to Lesser (2002) the crack initiation stage takes about 95% of the fatigue lifetime in the case of polymers. Sauer and Chen (1983) showed similar conclusions for high-impact polystyrene (HIPS) and polystyrene (PS). More recently, Janssen et al. (2008a) showed that based on their fatigue tests on samples of PC, polypropylene (PP), and PMMA, the initiation stage almost covers the entire fatigue life (>99%). Thus for many thermoplastics, the initiation of the crack should be considered in the modeling under fatigue loading. The failure criteria based approaches estimate the limit state for the material under fatigue loading, but they can’t handle realistic fatigue loadings directly. Moreover, they don’t allow to model the progressive failure until the crack initiation within the material. For this purpose, the use of sophisticated material behavior models such as in the work of Janssen et al. (2008a) is more justified. But the main limitation of these models is that the considered material failure mode is mainly ductile and related to macroscopic geometric effect such as necking. In the case of HCF loading, considered generally to be mechanically dominated, the material failure may be also brittle and sudden without important macroscopic deformation. As detailed in the introduction chapter, one explanation of this behavior is the effect of preexisting defects and inhomogeneities (Lesser, 2002) or low density domains of voids created during fatigue loading for TPs such as PA66 (Mouriglia-Seignobos et al., 2014). Thus we propose a multiscale approach modeling for TPs under HCF loading defined by a non-visible material deterioration at macro-scale and negligible thermal effects. The proposed approach should give a good estimation of the initiation of a crack responsible of final material failure. The details about our proposed model and its experimental evaluation are given in the following section.
4.2 Proposed modeling approach and its evaluation

4.2.1 Modeling approach

Based on the idea that damage occurs at localized zones within the material, it is assumed that the volume element were the fatigue failure may occur within the material is defined by an undamaged matrix with weak spots having ellipsoidal shapes. The weak spots correspond to existing defects or heterogeneities in the material. Figure 4.2.1, illustrates the proposed multiscale model.

The matrix behavior is assumed to be VE and the weak spots follow a VEVPD behavior. In order to predict the stresses and strains within each phase: matrix and weak spots, a mean field homogenization (MFH) model is proposed. The details about the developed MFH model are given in chapter 3.

![Multiscale damage model for homogeneous thermoplastic polymers materials.](image)

4.2.1.1 Main assumptions

The main assumptions of the modeling approach are the following:

- The failure of the material happens when the damage within the weak spots reaches a critical value: $D_{ws} > D_c$.
- The volume fraction of the weak-spots is assumed to be low. Its effect is assumed to be negligible at macroscale and macroscopically the material remains basically viscoelastic. However the damage evolves at the scale of the weak spots.
- At the level of weak spots, the isotropic hardening and kinematic hardening are neglected.
4.2 Proposed modeling approach and its evaluation

4.2.1.2 Numerical algorithm

The numerical algorithm proposed for MFH of two VEVPD phase composites, illustrated in figure 3.3.2, is used in the case of matrix assumed to be viscoelastic, which is a particular case of VEVPD behavior. The damage within the weak spots is estimated for each time increment. In order to check material failure, a failure criterion based on critical damage value is used. The numerical algorithm for the proposed model is summarized in the figure 4.2.2.

![Diagram of the numerical algorithm for the proposed model.](image)

Figure 4.2.2: Illustration of the numerical algorithm for the proposed model.

4.2.2 Experimental evaluation

The experimental results of (Berrehili, 2010; Berrehili et al., 2010a) on high-density polyethylene (HDPE) were employed in order to evaluate the proposed approach. Berrehili et al. investigated the multiaxial fatigue behavior of HDPE at room temperature and low frequency (≤ 2 Hz). According to the authors, performing their investigations at this frequency range allows to limit the influence of self heating on the material behavior, and the fatigue can be considered mainly mechanical. They used extruded pipes in order to avoid buckling in the case of negative loading ratio and to be able to apply multiaxial cyclic loading in tension, compression, and torsion. The fatigue tests are stress controlled.

4.2.2.1 Material parameters

The viscoelastic parameters for both the matrix and the weak spots are estimated using the tensile curves for different values of stress rates (cf. figure 4.2.3), since DMA test results for different values of the frequency are not provided. The parameters, listed in table 4.1, are used to simulate the VE behavior of the material under several stress rates in figure 4.2.3.
4.2 Proposed modeling approach and its evaluation

Figure 4.2.3: HDPE response under uniaxial tension under different strain rates. Symbols stand for experimental results from (Berrehili, 2010; Berrehili et al., 2010a,b)[Ref.1], Nguyen (2013)[Ref.2] and solid lines for numerical simulations with the VE model. Material parameters are listed in Table 4.1.

Table 4.1: VE parameters for the matrix and weak spots in HDPE at T=23°C, identified based on experimental results of (Berrehili, 2010).

<table>
<thead>
<tr>
<th>Initial modulus</th>
<th>$E_0=3000$ MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisson’s ratio</td>
<td>$\nu = 0.3$</td>
</tr>
<tr>
<td>$E_i$(MPa)</td>
<td>$\tau_i$(s)</td>
</tr>
<tr>
<td>981.5</td>
<td>0.01</td>
</tr>
<tr>
<td>611.0</td>
<td>0.36</td>
</tr>
<tr>
<td>500.0</td>
<td>80</td>
</tr>
</tbody>
</table>

The viscoplastic and damage parameters within the weak-spots are identified using S-N curve for fatigue tensile test at a loading ratio ($R=0$), by reverse engineering. The shape of the weak spots is chosen to be spherical. The weak spots volume fraction is taken as 2%, the best fit is plotted in figure 4.2.4. The parameters are listed in table 4.2.
4.2 Proposed modeling approach and its evaluation

Figure 4.2.4: S-N curves of HDPE under a tensile fatigue loading, at loading ratio $R=0$ and frequency $F=2\text{Hz}$. Solid line stand for the numerical simulation, symbols stand for experimental results and the arrow corresponds to stopped test without failure.

<table>
<thead>
<tr>
<th>Initial yield stress</th>
<th>$\sigma_y = 7 \text{MPa}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscoplastic function: $g_v = \frac{\sigma_y}{\eta} \left( \frac{f}{\sigma_y} \right)^m$</td>
<td></td>
</tr>
<tr>
<td>$\eta = 29.10^6 \text{MPa.s}$</td>
<td>$m = 6.2$</td>
</tr>
<tr>
<td>Damage function: $\dot{D} = \left( \frac{Y}{S_D} \right)^m \dot{\rho}$</td>
<td></td>
</tr>
<tr>
<td>$S_D = 0.02 \text{MPa}$</td>
<td>$s_D = 2.3$</td>
</tr>
<tr>
<td>$P_D = 0$</td>
<td>$D_c = 25%$</td>
</tr>
</tbody>
</table>

Table 4.2: VP parameters for weak spots in HDPE at $T=23^\circ\text{C}$, identified based on experimental results of (Berrehili, 2010).

The effect of the weak spots volume fraction ($v_{ws}$) is evaluated. Figure 4.2.5 shows S-N curve for fatigue tensile $R=0$ and frequency $F=2\text{Hz}$ for several values of $v_{ws}$: 10%, 2%, 1% and 0.5%. For values less than 2% the $v_{ws}$ has almost no influence on the fatigue failure behavior. It is seen that if the volume fraction of weak spots is less than 2%, and it has no effect on the macroscale. For all subsequent simulations, the $v_{ws}$ is considered to be less than 2%. It is known that in MFH techniques, the M-T method gives comparable results to the so-called dilute inclusion, in the case of a low volume fraction of inclusions (cf. chapter 3 for more details).
4.2 Proposed modeling approach and its evaluation

Figure 4.2.5: S-N curves of HDPE under a tensile fatigue loading, at loading ratio \( R=0 \) and frequency \( F = 2 \text{Hz} \), for different values of \( v_{ws} \). The material parameters are listed in the table 4.1.

### 4.2.2.2 Interaction between the matrix and the weak spots

The material is assumed to remain viscoelastic at the macroscale. However, at the weak-spots scale the behavior is VEVPD, and fatigue damage is evolving at that scale. Hereafter, the results of numerical simulation of a fatigue tensile test at a loading ratio \( R = 0 \), frequency \( F = 2 \text{Hz} \) and a maximum stress \( \sigma_{t1max} = 25 \text{MPa} \) as shown. The volume fraction of the weak spots is equal to 2%.

Figures 4.2.6 and 4.2.7 show respectively the stress and the strain within the matrix and the weak spots and all the material, for the first cycles of loading and last cycles before the final failure. For the first cycles, the state within the weak spots is similar to the state within the matrix and the overall material, whereas for the last cycles before final failure, the strain is higher because of increasing of the plastic accumulation (cf. figure 4.2.8) and the stress is lower because of the presence of the damage in the weak spots. The evolution of the plastic accumulation and the damage as a function of number of cycles within the w.s. are plotted in figure 4.2.8.
4.2 Proposed modeling approach and its evaluation

Figure 4.2.6: Stress as a function of time under cyclic loading at loading ratio $R=0$, frequency $F=2\, \text{Hz}$ and maximum stress $\sigma_{11\text{max}} = 25\, \text{MPa}$. 
4.2 Proposed modeling approach and its evaluation

Figure 4.2.7: Strain as a function of time under cyclic loading at loading ratio $R=0$, frequency $F = 2\,Hz$ and maximum stress $\sigma_{11\text{max}} = 25\,MPa$.

The effect of the variation of maximum stress on the fatigue damage evolution is shown in the figure 4.2.9. The level of applied macro-stress affects the damage evolution, thus the number of cycles to failure changes as a function of the applied load.
4.2 Proposed modeling approach and its evaluation

Figure 4.2.8: Plastic accumulation and damage in the weak spots as function of number of cycles at loading ratio $R=0$, frequency $F = 2\text{Hz}$ and maximum stress $\sigma_{11\text{max}} = 25\text{ MPa}$.

Figure 4.2.9: Damage in the weak spots vs. number of cycles for different values of maximum tensile macro-stress, within the weak spots under a tensile fatigue loading, at loading ratio $R=0$ and frequency $F = 2\text{Hz}$.

4.2.2.3 Effect of loading ratio and the frequency

Figure 4.2.10 shows the S-N curves obtained by the proposed model compared to experimental results of Berrehili et al. (2010a). The model gives a good
4.2 Proposed modeling approach and its evaluation

correlation with the experimental results and captures the mean stress effect and the change of the loading frequency. As shown by the experimental results, the S-N curves in the case of fatigue tension and compression are similar. In the proposed model, pressure doesn’t have important effect on the response. Therefore the predicted failure is not sensitive enough to pressure, although the evolution of damage depends on the pressure via the damage thermodynamic force \( Y \). Hence the S-N curves in tension and in compression are superposed which is consistent with the experimental data.

![S-N Curves](image)

**Figure 4.2.10:** S-N curves of HDPE under tension and compression fatigue loadings, at different loading ratios and frequencies. Model predictions (lines) compared to experimental data of Berrehili et al. (2010a)- symbols. Arrows correspond to stopped tests without failure.

4.2.2.4 Effect of multiaxial loadings

The model is also used to predict the S-N curves under torsion, and compared to the experimental results from Berrehili et al. (2010a). The results of the numerical simulations are shown in figure 4.2.11, they have a good agreement with the experimental results. We emphasize that all numerical simulations are done with the same set of parameters, given in table 4.1 and 4.2 and a weak spots volume fraction of 2%.

4.2.2.5 Influence of the stress signal shape

The change of shape of the stress signal has an influence on the model predictions as shown in the figure 4.2.12. The sinusoidal signal leads to shorter life time than the triangular signal. These sensitivity is not captured by several modeling approaches such as stress based criteria.
4.2 Proposed modeling approach and its evaluation

Figure 4.2.11: S-N curves of HDPE under tension, compression and torsion fatigue loadings, at different loading ratios and frequencies. Model predictions (lines) compared to experimental data of Berrehili et al. (2010a)- symbols. Arrows correspond to stopped tests without failure.

Figure 4.2.12: Predicted S-N curves of HDPE under a tension fatigue loading, two different type of signal stress shape.
4.3 Discussion and possible enhancements

The proposed model showed good capabilities to capture the main effects observed experimentally, which are the mean stress effect and the sensitivity to multiaxial loading. But some enhancements need to be done in order to better capture these effects. The model may be also used or extended to be applied in other cases. In the following these possibilities are listed.

Mean stress effect Possible enhancement in order to better capture the mean stress may be accomplished by using a different yield function which separates the viscoelastic and the viscoplastic behavior within the weak spots. For metals, similar approach based on localized fatigue damage does exist (eg. Lemaitre and Doghri, 1994; Lemaitre et al., 1999; Desmorat et al., 2007) where the damaged zones have an EP damaged behavior, but they could not be used for TPs since they don’t take into account the effect of viscosity. The strain concentration laws are also different. This approach suffer of the insensitive to the loading ratio, recently Desmorat et al. (2015) proposed different approach to to capture this sensitivity for metals by using several yield functions for the EP behavior of metals.

Time increment effect From a numerical point of view, the time increment for each time step seems to have an important influence on the results. The history dependence taken into account by the model is one reason for this sensitivity. In order to choose the most suitable time increment per cycle, a parametric study was performed and the results are shown in figure 4.3.1. The tests were performed under several time increments per cycle: 8, 20, 50 and 100. As shown, the sensitivity is not important for a sufficient number of time increments per cycle. A fast estimation of the model results may then be performed using few increments per cycle.

In other hand, the time of computation may be reduced by using a time homogenization method, as the method proposed by Haouala and Doghri (2015).

Low cycle fatigue For low cycle fatigue, defined by high frequency or high level of applied mechanical loading, a macroscale approach such as the Janssen et al. (2008b) approach is more suitable than the weak spots concepts. The proposed VEVPD model may be used at the macroscale for this purpose, however a modification is needed in order to take into account self heating (cf. chapter 6).

Anisotropic fatigue damage For some TPs, the fatigue damage may be considered to be anisotropic. The presented model may be employed in this case by considering that the shape of the weak spots is ellipsoidal and their orientation is not 3D-random. Numerical simulations with the model using several aspect ratios, under tensile fatigue applied in the main direction and the longitudinal direction of the weak spots for different values of aspect ratio, are shown in figure 4.3.2. The S-N curves predicted by the model showed the
4.3 Discussion and possible enhancements

sensitivity of the model to the direction of the applied loading, when the aspect ratio $A_r$ is different from 1.

Figure 4.3.1: S-N curves of HDPE under a tensile fatigue loading, at $R=0$ and frequency $F=2$ Hz, for different values of number of increment per cycle.

Figure 4.3.2: S-N curves of HDPE under a tensile fatigue loading for different values of aspect ratio. The loading is applied on the longitudinal and transverse direction of the aligned weak spots.
4.4 Conclusion

Throughout this chapter an overview of the existing literature on the fatigue modeling of thermoplastic polymers was presented. Our proposed model which may be classified as a crack initiation based approach was discussed and its originality was highlighted. An experimental validation was performed against the results of fatigue tests carried out on HDPE from Berrehili et al. (2010a). Our proposal showed a good capability to capture the main effects observed experimentally such as the effects of multiaxial loading and the sensitivity to the loading ratio. Possible enhancements are discussed in section 4.3 in order to enlarge the field of application of the proposed model. In addition, it was shown that possible anisotropy of the material fatigue failure may be taken into account by changing the aspect ratio and the orientation of the weak spots.
Chapter 5

A multiscale model for the high cycle fatigue of SFRTPs

Based on experimental observations presented in the introductory chapter about the failure of SFRTPs, a multiscale modeling approach is proposed. In this chapter, this approach is detailed and evaluated, against experimental fatigue tests on SGFPA66 performed within the DURAFIP project framework. A review about the existing modeling approaches is presented in section 5.1 in order to highlight the originality and the advantages of the proposed approach.

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5.1 State-of-the-art description

The modeling of SFRTPs mainly under regular service loading, has been an active research field during the last decade. However, the failure behavior under fatigue loading was much less studied. The majority of the proposed approaches make use of the huge experience on modeling of classical materials such as metals. The material was considered either as anisotropic and homogeneous, then modeled at the macroscopic scale, or the microstructure was taken into account in different ways. Taking into account the effect of SFRTPs complex microstructure was studied in several works, mainly in order to predict the thermo-elastic material properties. A realistic approach has to be based on a good estimation of the fiber orientation using for example the concept of orientation tensor (e.g., Advani and Tucker III, 1987; Doghri and Tinel, 2006). SFRTPs at a given loading level are characterized also by an irreversible and loading rate dependent behavior generally called viscoplastic, which motivated several modeling works such as (e.g., Kammoun et al., 2011a; Brassart et al., 2011; Miled et al., 2013).

Similar to unreinforced TPs, the lifetime of SFRTPs can be defined by two stages: initiation stage and propagation stage, according to Klimkeit et al. (2011a) who worked on short fiber reinforced PBT+ PET and Noda et al. (2001) who worked on short glass-fiber reinforced nylon 66, the propagation stage occurs very rapidly after the initiation stages and the former may define the whole lifetime of the material.

In this section the focus is on the main existing modeling approaches of SFRTPs under fatigue loading, based on the crack initiation prediction. The crack propagation based approaches are using fracture mechanics, as detailed in the previous chapter. The selected modeling approaches may be classified in two categories: failure criteria based approaches and progressive failure based approaches.

5.1.1 Failure criteria based approaches

Several approaches based on failure criteria are proposed in the literature, mainly inspired from the existing criteria for metals. The classical existing criteria are different for low and high cycle fatigue, as explained in section 4.1. However, since no visible distinction between LCF and HCF for SFRTPs is generally observed, they are usually used in all cases of fatigue loadings without distinction. As shown in the introduction chapter the material anisotropy, due to the FOD and FLD, plays an important role in fatigue failure. Thus, classical criteria used for metals assumed to be homogenous and isotropic will not be predictive. Hence some authors tried to include the anisotropy in a phenomenological way in order to be able to use such criteria (e.g., Launay et al. (2013b)).

In the work of Launay et al. (2013b,a), several criteria inspired from the existing classic ones were employed, based on a steady (or stabilized) state given by a nonlinear constitutive model for cyclic behavior of SFRPA.66 (Launay et al., 2011b). The constitutive model was developed in the framework of finite strain elasto-viscoplasticity, taking into account the fiber directions. Using
physical quantities, computed by the model at stabilized state (estimated at 20 cycles), the criteria predictions were compared to the published results of Klimkeit et al. (2011b) and De Monte et al. (2010a) on specimens made out of polyamide 66 reinforced with 35% of short glass fibres. Both studies are performed at room temperature, with material conditioned at equilibrium with air containing 50% of relative humidity (RH50) or dry-as-moulded (DAM). Other earlier works applied some of the existing criteria such as Klimkeit et al. (2011b) and Bernasconi et al. (2007). Hereafter, the main criteria\footnote{Some of the criteria were already listed in the last chapter. Since they were modified in the SFRTPs fatigue context, they are listed again in this chapter}, employed for fatigue of SFRTPs, are listed. The conclusions of the authors based on their comparison with experimental results, are reported as well.

5.1.1.1 Stress based failure criteria

**Shear stress criterion**  It is called this way, because it uses as stress measure the octahedral shear-stress intensity. Launay et al. (2013b) used the von Mises norm (cf. eq. 5.1.1) and the anisotropic Hill norm (cf. eq. 5.1.2), in order to measure the radius of the smallest hypersphere circumscribing the loading path in the 5-dimension deviatoric stress space :

\[
J_{2,VM}^a = \min_{s_1} \max_{t \in [0, T_{cycle}]} \left\{ \frac{1}{2} \left( s_1 - s(t) \right) : \left( s_1 - s(t) \right) \right\} \tag{5.1.1}
\]

\[
J_{2,Hill}^a = \min_{s_1} \max_{t \in [0, T_{cycle}]} \left\{ \frac{1}{2} \left( s_1 - s(t) \right) : P : \left( s_1 - s(t) \right) \right\} \tag{5.1.2}
\]

where \(P\) is the Hill tensor which is a fourth-order tensor introduced to generalize the von Mises (isotropic) equivalent stress to anisotropic microstructure.

The major drawback of these criteria is that they are pressure insensitive. And as shown by Klimkeit (2009) and Launay et al. (2013b), they are not able to capture the mean stress effect. In order to test whether or not the mean stress effect is due to the hydrostatic stress change other criteria, considered to be pressure dependent, are employed.

**Criteria based on shear stress and hydrostatic stress**  Inspired by the Crossland, Sines and Van Dang criteria (Van Dang et al., 2001; Constantinescu et al., 2003; Fares et al., 2006), Launay et al. (2013b) proposed the following criteria, respectively:

\[
\sigma_{eq.Cr} = J_{2}^a(\sigma) + \alpha P_{max} \tag{5.1.3}
\]

\[
\sigma_{eq.Si} = J_{2}^a(\sigma) + \alpha P_{avg} \tag{5.1.4}
\]

\[
\sigma_{eq.DV} = \max_n \max_t \left[ \tau(\vec{n}, t) + \alpha P_{max}(t) \right] \tag{5.1.5}
\]

where \(J_{2}^a\) is defined using eq.5.1.1 or eq.5.1.2, \(P_{max}\) and \(P_{avg}\) are respectively the maximum and the average of the hydrostatic stress over the stabilized cycle. The Van Dang criterion allows to find the material orientation \(\vec{n}\) which is subjected to the highest shear \(\tau\).

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Principal stress The principal stress was used by Klimkeit (2009) and Launay et al. (2013b). However, the expression was extended from monotonic static to fatigue loadings differently. Klimkeit (2009) used only the component of the amplitude stress in the plane of the studied specimen. Launay et al. (2013b) formulated a criterion with the amplitude of the highest stress eigenvalue $\sigma_{\text{princ}}$ over the stabilized cycle given by their constitutive model.

Modified Tsai-Hill criteria As indicated by their designation, they are derived from the original Tsai-Hill criterion (cf. Appendix D for more details about the original formulation), because of its successes to predict the failure of unidirectional continuous fiber reinforced composites under monotonic static loading, several versions of the Tsai-Hill criterion, were proposed, in order to predict the fatigue failure of SFRTPs (e.g., Zago and Springer, 2001a; Bernasconi et al., 2007; De Monte et al., 2010b; Klimkeit et al., 2011a; Launay et al., 2013b).

The observed layered structure of the SFRTPs microstructure, motivated the use of the plane (2D) version of the criterion ($i_3 = 0$, $i = \{1, 3\}$). As modified in some works (e.g., Bernasconi et al., 2007; De Monte et al., 2010b), the static strengths in the original formulation were replaced by Basquin equations as a function of the number of cycles to failure ($N_r$). The modified criterion is then expressed as:

$$
\left( \frac{\sigma_{11}}{S_1(N_r)} \right)^2 + \left( \frac{\sigma_{22}}{S_2(N_r)} \right)^2 - \frac{\sigma_{11}\sigma_{22}}{S_2^2(N_r)} + 2 \left( \frac{\sigma_{12}}{T_1(N_r)} \right)^2 = 1 \quad (5.1.6)
$$

with $S_1(N_r) = S_{1r}^0 N_r^{-1/\beta_1}$, $S_2(N_r) = S_{2r}^0 N_r^{-1/\beta_2}$ and $T_1(N_r) = T_{1r}^0 N_r^{-1/\alpha_1}$. The material parameters $S_{1r}^0$, $\beta_1$, $S_{2r}^0$, $\beta_2$, $T_{1r}^0$ and $\alpha_1$ are identified using S-N curves. The results of Bernasconi et al. (2007); De Monte et al. (2010b) showed much more ability to take into account the microstructure of the studied samples, compared to the other criteria. However, the following limitations still exist: the insensitivity to the mean stress effect and to a change of microstructure because its coefficients are identified for a given microstructure. This leads to limitations in terms of industrial application.

In order to overcome these limitations Launay et al. (2013b) modified the Tsai-Hill criterion by employing the orientation tensor $\alpha^0$, and proposed a new version of the criterion. They modified the fourth-rank symmetric tensor $M$, containing the material parameters used in Tsai-Hill criterion in the general 3D case (cf. Appendix D for details), by the following expression:

$$
M(\alpha^0) = a_1 M_1 + a_2 M_2 + a_3 M_3 \quad (5.1.7)
$$

where $a_i$ are the principal values of the orientation tensor, and $M_i$, associated with a unidirectional microstructure along $\tilde{u}_i$, $i \in \{1, 2, 3\}$, are expressed by:
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\[
M_i = \begin{bmatrix}
\frac{1}{\sigma_{\text{long}} - 0.5 \sigma_{\text{long}}} & \frac{1}{\sigma_{\text{transv}} - 0.5 \sigma_{\text{long}}} & 0 \\
\frac{1}{\sigma_{\text{long}} - 0.5 \sigma_{\text{long}}} & \frac{1}{\sigma_{\text{transv}} - 0.5 \sigma_{\text{long}}} & 0 \\
\frac{1}{\sigma_{\text{long}} - 0.5 \sigma_{\text{long}}} & \frac{1}{\sigma_{\text{transv}} - 0.5 \sigma_{\text{long}}} & 0 \\
s\text{sym} & 0 & 0 \\
\end{bmatrix}
\]

(5.1.8)

\[M_2 \text{ and } M_3 \text{ are composed by the same material parameters (}\sigma_{\text{long}}, \sigma_{\text{transv}}\text{ and } \tau_{\text{long}}\text{)}\text{ as } M_1\text{, but differ by rotations. Finally, similar to the other stress criteria, the physical quantity that was chosen to be used in their criterion is the following:}

\[G^b_{\text{sym}} = \min_{\sigma_1} \max_{t \in [0,T_{\text{cycle}}]} \left\{ \sqrt{\left( \sigma_1 - s(t) \right) : M(a^p) : (\sigma_1 - s(t))} \right\}
\]

(5.1.9)

5.1.1.2 Strain and energy based failure criteria

**Manson-Coffin criteria** The Manson-Coffin model, usually used for LCF of homogenous metals, was modified by Launay et al. (2013b) using the amplitude of (visco-)plastic strain along the loading direction during a cycle \(\varepsilon_{\text{vp}}^a\), given by their model, instead of the plastic deformation. The original Manson-Coffin was extended to multiaxial loadings case as follows:

\[\varepsilon_{\text{vp}}^a (N_v)^b = C \]

(5.1.10)

where \(b\) and \(C\) are material parameters. And \(\varepsilon_{\text{vp}}^a\) is obtained by measuring the radius of the smallest hypersphere circumscribing the loading path in the 5-dimension plastic strain space:

\[\varepsilon_{\text{vp}}^a = \min_{\varepsilon_1} \max_{t \in [0,T_{\text{cycle}}]} \left\{ \sqrt{\frac{2}{3} (\varepsilon_1 - \varepsilon_{\text{vp}}(t)) : (\varepsilon_1 - \varepsilon_{\text{vp}}(t))} \right\}
\]

(5.1.11)

**Energy based criteria** Klimkeit et al. (2011b) proposed to use the density of elastic strain energy, and found that it gives a good correlation to fatigue life. They were inspired by the work of Kujawski and Ellyin (1995) which takes into account mean-stress effects. Launay et al. (2013b) also modified the existing energy based criteria, in order to be more suitable to their studied material. According to their constitutive model, the dissipated energy can be expressed by three parts of the instantaneous dissipation integrated over one cycle: the viscoelastic dissipation (\(\Delta W_{\text{ve}}\)), the viscoplastic dissipation (\(\Delta W_{\text{vp}}\)) and a softening dissipation (\(\Delta W_s\)) assumed to be negligible for the stabilized cycle. So they expressed this criterion as:

\[(\Delta W_{\text{vp}} + \alpha \Delta W_{\text{ve}}) \cdot N_v^b = C \]

(5.1.12)

where \(a\), \(b\) and \(C\) are material parameters. The energy based criterion proposed by Launay et al. (2013b) showed a better prediction compared to the majority of criteria presented in this section, according to their comparison against
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Experimental results, mainly performed on standard samples and published by Klimkeit et al. (2011b) and De Monte et al. (2010a). A further validation for a real workpiece and real loading has to be made in order to validate the correlation found with these criteria.

Although the failure criteria based approaches can lead to satisfactory results in terms of prediction of the S-N curves of laboratory specimens, their use is still complicated for industrial purposes, on real workpieces. Their major limitations are that they can’t handle a complex history of fatigue loading, and they can’t model the observed progressive failure of the material, commonly called progressive damage.

5.1.2 Progressive failure based approaches

In order to measure progressive failure, several variables were employed. The most common one is the hysteresis loops. The change of their slope is usually considered as an indicator of progressive failure. Several measurable mechanical quantities related mainly to the stress strain curves were employed to plot the damage evolution, such as the hysteresis loop, strain energy, and hysteresis energy dissipation (see figure 5.1.1). From a modeling point of view a scalar damage variable is employed when the material is assumed to be isotropic. Such is the case of (Wang and Chim, 1983) who worked on a random short-fiber SMC composite, and expressed the damage as:

\[
\begin{align*}
D &= 1 - \frac{E}{E_0} \\
\frac{dD}{dN_r} &= A(D) N_b^b 
\end{align*}
\]  

(5.1.13)

where \(E_0\) and \(E\) are the initial and current hysteresis loop slopes, respectively. \(A(D)\) is a function of the damage variable \(D\) and \(b\) is a material parameter.

Figure 5.1.1: Schematic presentation of the different parameters employed to capture damage evolution.
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A more sophisticated modeling approaches, based on damage mechanics, were also used for SFRTPs progressive failure of the material, such as the model of Nouri et al. (2009) which takes the material anisotropy in a macroscopic way. Since the microstructure represents a layered-like configuration, the approach of (Ladèvéze and LeDantec, 1992) developed for laminate continuous fiber composites within the framework of continuum damage mechanics, was employed with a modification of the damage evolution law. They noticed that the first stage of damage is observed at the beginning of the loading, which is not taken into account by the original model. The authors based their approach on the following failure scenario, proposed by Van Paepegem and Degrieck (2002) (cf. a schematic presentation in the figure 5.1.2):

![Diagram of damage evolution](image)

- **Stage 1:** This stage corresponds to the onset of “damage zones”, which contain matrix micro-cracks and other forms of damage, such as matrix micro-voids. Hence, damage starts very early after a low number of loading cycles. It gives rise to an initial high stiffness reduction of the composite material,

- **Stage 2:** This stage corresponds to the coalescence and the propagation of the micro-discontinuities created during the first stage. The propagation occurs notably at the fibre–matrix interface zones. A gradual stiffness reduction of the material is then observed. This stage is a behavior accommodation and is characterized by a relative steady reduction of the composite stiffness as a function of cycle number.

- **Stage 3:** It corresponds to the last stage and is characterized by a dramatic damage accumulation due to the appearance of fibre fracture and
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...macroscopic crack propagation. The third damage stage may result in a rapid stiffness reduction leading to total material failure.

In the model of Nouri et al. (2009), the material behavior is assumed to be an elastic and anisotropic behavior and the damage is introduced through five internal state variables, coupled with elastic behavior, defined as follows:

\[
\begin{cases}
E_i = E_i^0 (1 - d_{ii}) ; & \text{for } (i = 1, 2) \quad \text{(no sum)} \\
G_{ij} = G_{ij}^0 (1 - d_{ij}) ; & \text{for } (i \neq j; i, j = 1, 2, 3) \quad \text{(no sum)}
\end{cases}
\]

(5.1.14)

where \(E_i\) \((i = 1, 2)\) are damaged longitudinal (direction 1) and transverse (direction 2), \(G_{ij}\) \((i \neq j; i, j = 1, 2, 3)\) are in-plane and transverse shear moduli. The damage variables \(d_{ij}\) \((i \neq j; i, j = 1, 2, 3)\) are the damage variables.

The considered elastic energy of the damaged material is given by the following expression

\[
2W_d = \sum_{(i \neq j; i,j=1,2)} \frac{1}{1 - \nu_{ij}\nu_{ji}} \left[ E_i \varepsilon_{ii} \epsilon_{ii} + \nu_{ij}\epsilon_{jj}\right]_+ + E_i^0 \varepsilon_{ii} \epsilon_{ii} + \nu_{ij}\epsilon_{jj}\right]_-
\]

\[
+ \sum_{(i \neq j; i,j=1,2,3)} G_{ij} \gamma_{ij}^2
\]

(5.1.15)

where \((\cdot)_+\) and \((\cdot)_-\) stand for the positive and negative parts of \((\cdot)\), respectively. It assumes that under compressive loading, transverse matrix cracks are supposed to be closed up and do not have any influence on the damage evolution, but they are active in the case of tension.

The thermodynamic dual variables \(Y_{ij}\) \((i, j = 1, 2, 3)\) associated to the damage variables \(d_{ij}\) are derived from the strain energy \((W_d)\) of the damaged material, as given by following relations

\[
\begin{cases}
Y_{ii} = -\frac{\partial W_d}{\partial d_{ii}} = \frac{1}{2} \frac{1}{1 - \nu_{ij}\nu_{ji}} E_i^0 \varepsilon_{ii} \epsilon_{ii} + \nu_{ij}\epsilon_{jj}\right]_+ ; & \text{for } (i \neq j; i, j = 1, 2)
\\
Y_{ij} = -\frac{\partial W_d}{\partial d_{ij}} = \frac{1}{2} G_{ij} \gamma_{ij}^2 ; & \text{for } (i \neq j; i, j = 1, 2, 3)
\end{cases}
\]

(5.1.16)

The damage evolution law are expressed as function of the number of cycles and the \(Y_{ij}(i, j = 1, 2, 3)\) as:

\[
\frac{\partial d_{ij}}{\partial N} = \frac{\alpha_{ij}\beta_{ij}}{1 + \beta_{ij}} (Y_{ij})^{\beta_{ij}-1} + \lambda_{ij} Y_{ij} \exp (-\delta_{ij} N) \quad (i, j = 1, 2, 3, \text{ and no summation})
\]

(5.1.17)

Where \(\alpha_{ij}, \beta_{ij}\) and \(\delta_{ij}\) are the 15 material parameters to be identified. The Nouri et al. (2009) model was used to reproduce the experimental damage of SGFRPA.6 under loading ratio equal to 0.3 (Nouri et al., 2009; Meraghni et al., 2011). Meraghni et al. (2011) gave a formulation for in-plane damage involving three variables: \(d_{11}, d_{22}\) and \(d_{12}\).
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The major limitation of this type of approach is the insensitivity to microstructure change and to the loading rate, and it is difficult to be used in the case of real complex loading. Another critique is about the measure of damage during loading, since the very low thermal conductivity of the polymer material together with the viscous part of its behavior, make it very sensitive to changes in temperature. The change of slope can be a result of self heating which can be important and may introduce a loss of stiffness of the material, but which is not necessarily irreversible. However the loss of stiffness due to mechanical fatigue is irreversible since it is related to the irreversible deformations. In conclusion, measuring the damage based on the change of the hysteresis loops slope is not a reliable measure.

5.1.3 Summary

In summary, the failure criterion based approaches, can only estimate the limit state of the material failure. Few of them take into account the effect of the microstructure, but in a phenomenological way. They can’t model the progressive damage of the material under fatigue. Although the existing progressive failure models try to reproduce the loss of stiffness of the materials, for a given microstructure, the change in the microstructure is not captured without identifying a new set of material parameters.

There is a need to develop a multiscale approach in order to reproduce the observed damage mechanisms, to take into account the complex microstructure and handle complex loadings, which will make the modeling of real workpieces and their design easier. This is the motivation of the present work. Our objective is to propose a modeling approach that is able to reproduce the real behavior of the material based on physical considerations. The problem is too complex, and a lot of work needs to be done in order to obtain a reliable modeling approach. However, recent developments of multiscale approaches either with full-field computations or mean-field homogenization techniques, gives some clues to a possible solution. An example of this work is that of Spahn and Linder (2015), who performed a FE computation of PA matrix reinforced with GF. The matrix is assumed to have a damaged elastic behavior. Although this kind of model does not fully describe the behavior of the material, it is able reproduce some experimental observations. Figures 5.1.3 give an example of their results.

Another possibility is by using homogenization techniques such as mean field homogenization. Several models showed a successful prediction of the SFRTPs behavior under monotonic loading. One can cite the work of (Kammoun et al., 2011b, 2015) based on using the concept of pseudo-grains (PG) together with the orientation tensor and a two-step homogenization (cf. figure 5.1.4), they were able to predict successfully the behavior of PA 66 reinforced with several volume fractions of GF under monotonic loading and others loading cases. Two approaches were proposed both applied at the level of the PGs, one using failure criterion and called FPGF and the other using damage mechanics (FPGD).
5.1 State-of-the-art description

Figure 5.1.3: (a) Maximum damage values in the 90° sample after monotonic loading, (b) Experimental and simulated cyclic stress strain curves for an angle of 90°. Numerical results obtained by FE computation from Spahn and Linder (2015).

Figure 5.1.4: Schematic illustration of the FPGF model. Instead of the real RVE, a numerical RVE is studied, which is a discrete set of Unidirectional (UD) "Pseudograins" (PGs). In the two-step homogenization procedure, each pseudograin is homogenized in the first step, and the effective response of the set of homogenized PGs is computed in the second step. Failure is checked for each individual PG. When a PG fails, its incremental contribution to the overall RVE’s response is eliminated or reduced. (From Kammoun et al., 2011b).
5.2 Proposed modeling approach and its evaluation

5.2.1 Proposed modeling approach

In this section a modeling approach similar to the previous one for fatigue of TPs \( (\text{cf. chapter 4}) \) is proposed for SFRTPs. Based on the concept of weak spots in SFRTPs, damaged zones assumed to be the origin of the macro-crack initiation in SFRTPs are considered. Those weak spots may be created at the interface between the matrix and the fibers. Indeed the stiffness contrast between the two types of materials induces some stress concentration regions especially at fibers tips. Within those regions irreversible deformation and damage may occur, as detailed in chapter 1 \( (\text{cf. also figure 5.1.3 for a damaged elasto-plastic PA matrix reinforced with GF under cyclic loading}) \). The weak spots also model the preexisting defects or inhomogeneities within the matrix.

In the proposed model, the material microstructure is defined by the following phases:

1. An undamaged TP matrix assumed to obey a linear viscoelastic model
2. Misaligned fibers assumed to be elastic
3. Weak spots which obey a VEVPD material behavior.

In order to measure the interaction between those phases and obtain an estimate of the average state within each phase, mean field homogenization method is chosen. The main limitation of considering a three phase composite in this case is the lack of information about the geometries of the weak spots and their volume fraction. Besides, computation time for homogenization under fatigue loading is expensive.

Also similarly to the model for fatigue of TPs, the volume fraction of the weak spots is considered to be small, thus it has a negligible effect on macroscale response and on the interaction between the TP matrix and the misaligned fibers. By considering this assumption, an uncoupled problem is formulated and will be detailed hereafter.

The proposed uncoupled approach \( (\text{cf. Figure 5.2.1}) \) is based on the idea of separating the behavior at the macroscale and the behavior at the level of weak spots. The loading applied on the weak spots, assumed to obey a VEVPD model, is given by the behavior of the VE matrix reinforced with misaligned elastic short fibers. An example of weak spots loading, which is used in the presented numerical simulations is the mean strain within the matrix.
5.2 Proposed modeling approach and its evaluation

The main hypotheses of the proposed modeling approach are the following:

- The model is applied in the case of HCF loading, which is defined by a low level of loading (stress or strain) and low frequency.

- The interface between the matrix and the fibers is assumed to be perfect. However, generally this interface is treated in order to have good bonding between the two materials as it is explained in the introduction chapter. This treatment may create a new phase in the material having different behavior compared to the matrix and the fibers, thus the fiber will contribute to the macroscale behavior, only based on the loading transferred by this interface, which is less rigid than the fiber. In this work a reduction of the fibers’ elastic properties of the fibers is considered in order to take into account this effect.

- The material’s lifetime is assumed to be defined completely by the crack initiation stage, the crack propagation stage is neglected.

- The debonding between fibers and matrix is assumed to happen at the last stage of the material lifetime as part of the crack propagation stage. It is not considered in the modeling approach.

- Isotropic and kinematic hardenings are neglected within the weak-spots.

In order to take into account fiber orientation, the pseudo grain decomposition as in Kamoun et al. (2011b, 2015) is used. More details about this method are given in chapter 3. The PG decomposition is based on a two step homogenization method. At each time increment, the first step is the homogenization of each PG, which is composed of a VE matrix and unidirectional identical fibers, using an incrementally affine MT scheme proposed in chapter 3 for VEVPD.
two phase composites. The behavior of the PG is a particular case of VEVPD composites. The second step is homogenization of all the PGs using Voigt scheme.

5.2.2 Experimental evaluation

The proposed modeling approach is evaluated using experimental results for PA66 reinforced with 30% mass fraction of glass fibers, provided by our DU-RAFIP project partners. Specimens used for mechanical tests were machined from a rectangular plate produced by injection molding. They were cut-out at different angles w.r.t. the main flow direction (MFD) (0°, 45° and 90°) (cf. figure 1.2.4).

5.2.2.1 Modeling parameters

PA66 matrix  The matrix is assumed to obey a VE behavior. The VE parameters of the matrix are identified using a DMA test performed on unreinforced PA66 (see Figure 5.2.2), more details about the identification procedure are given in Appendix C. The choice of the number of relaxation times is related to the frequency range that the workpiece will be subjected to and the considered time of observation. Initial temperatures of the specimen are between 25°C and 30°C, then the identification is made for an average temperature between these two temperatures. The identified viscoelastic parameters are listed in table 5.1. The value of Poisson’s ratio ($\nu$) is assumed to be constant (cf. remarks in section 2.3.1).

Figure 5.2.2: Experimental (symbol) and analytical (solid lines) results of storage and loss moduli for PA66 RH50
5.2 Proposed modeling approach and its evaluation

Initial Young’s modulus

\[ E_0 = 2450 \text{ MPa} \]

Poisson’s ratio \( \nu = 0.35 \)

<table>
<thead>
<tr>
<th>( i )</th>
<th>( E_i (\text{MPa}) )</th>
<th>( \tau_i (\text{s}) )</th>
</tr>
</thead>
<tbody>
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<tr>
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<td>365</td>
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<tr>
<td>3</td>
<td>322</td>
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<td>1000000</td>
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<tr>
<td>10</td>
<td>24</td>
<td>1000000</td>
</tr>
</tbody>
</table>

Table 5.1: Linear viscoelastic parameters for PA66 RH50 identified from dynamic tests (cf. Figure 5.2.2).

Glass fibers In order to take into account the interface between the fiber and the matrix, a reduction of the elastic properties of the fibers, compared to standard parameters was considered. This enables a better correlation with the experimental results, as it is shown in the next subsection. The Young’s modulus is assumed to be equal to 28 GPa and the Poisson ratio is 0.22.

weak spots For the weak spots the same VE material parameters as for the matrix are considered. Viscoplastic and damage material parameters are identified using S-N curves by reverse engineering. As mentioned the isotropic hardening is neglected. The yield stress is considered to have a very low based on the assumption that the fatigue damage will start from the beginning of fatigue loading.

Fiber orientation As shown in the introduction, the material was studied by other authors such as Arif et al. (2014b), in the framework of DURAFIP project, with a special focus on the microstructure. A shown in figure 1.2.3, the orientation of fibers seems to be uniform in the so-called shell and core region, but random in the transition region. For our study as in Kammoun et al. (2011b, 2015), the average of orientation tensor over the specimen thickness is employed. And the weights of pseudo-grains representing different fiber orientations relative to the MFD presented in figure 3.4.3, are used.

5.2.2.2 The macroscale behavior under fatigue loading

The macroscale behavior is obtained using a two-step homogenization method based on a pseudo-grain decomposition. The first homogenization is performed
5.2 Proposed modeling approach and its evaluation

using MT scheme based on incrementally affine homogenization and the second one is performed using Voigt scheme.

The experimental tests are made at stress controlled test, the applied stress has a sinusoidal shape with a frequency of 3 Hz and a loading ratio R=0.1. As already mentioned, the fatigue tests were performed using specimens that were cut-out at different angles w.r.t. the flow direction (0°, 45° and 90°).

Hereafter, the advantage of employing the pseudo-grain decomposition instead of considering aligned assumption is highlighted. The comparison is made for the fist few cycles of the loading. 36 pseudo-grains are employed in the following simulations, as given in figure 3.4.3. In figures 5.2.5, 5.2.4 and 5.2.3, the numerical results, represented by continuous and dashed lines, are obtained under the two different assumptions and symbols stand for experimental data.

The results are normalized for confidentiality reason. The numerical simulations showed that by employing the PG decomposition the predictions are closer to the experimental results compared to considering the aligned fibers assumption.

![Figure 5.2.3: Numerical and experimental strain versus time curves, under a loading with maximum stress \( \sigma_{11_{\max}} = 0.45 \sigma_0 \) applied at 90° angle w.r.t. MFD.](image)

Figure 5.2.3: Numerical and experimental strain versus time curves, under a loading with maximum stress \( \sigma_{11_{\max}} = 0.45 \sigma_0 \) applied at 90° angle w.r.t. MFD.
5.2 Proposed modeling approach and its evaluation

When using the pseudo-grain decomposition method, the number of pseudo-grains (PGs) may have an important effect on the predictions accuracy. Hereafter a parametric study using the number of PGs is made in order to find the smallest possible number which allows to obtain acceptable predictions. Similar to the previous simulations, only few cycles are considered. The number of PGs considered in the study are 36, 19, 10, 6. The numerical simulations were made for the same three angles considered previously. The results are plotted in figures 5.2.6, 5.2.7 and 5.2.8. Except for the case of 6 pseudo-grains, all the others numbers give almost identical results. Thus for all the following simulations, only 10 pseudo-grains are used, in order to reduce the computation
5.2 Proposed modeling approach and its evaluation

Figure 5.2.6: Numerical strain versus time curves for different numbers of PGs, under a loading with maximum stress $\sigma_{11max} = 0.45\sigma_0$ applied at 90° angle w.r.t. MFD.

Figure 5.2.7: Numerical strain versus time curves for different numbers of PGs, under a loading with maximum stress $\sigma_{11max} = 0.52\sigma_0$ applied at 45° angle w.r.t. MFD.
5.2 Proposed modeling approach and its evaluation

Figure 5.2.8: Numerical strain versus time curves for different numbers of PGs, under a loading with maximum stress $\sigma_{11\text{max}} = 0.8\sigma_0$ applied at 0° angle w.r.t. to MFD.

Hereafter the numerical simulations in the case of large numbers of cycles are presented in figures 5.2.10, 5.2.9 and 5.2.11, respectively for the direction 90°, 45° and 0°, in terms of maximum strain as a function of the number of cycles.

Figure 5.2.9: Experimental and numerical maximum uniaxial strain vs. number of cycles, under fatigue loadings with maximum stress $\sigma_{11\text{max}} = 0.47\sigma_0$ and $\sigma_{11\text{max}} = 0.65\sigma_0$ applied at 90° angle w.r.t. MFD.
5.2 Proposed modeling approach and its evaluation

Figure 5.2.10: Experimental and numerical maximum uniaxial strain vs. number of cycles, under fatigue loadings with maximum stress $\sigma_{11\text{max}}=0.54\sigma_0$ and $\sigma_{11\text{max}}=0.70\sigma_0$ applied at $45^\circ$ angle w.r.t. MFD.

Figure 5.2.11: Experimental and numerical maximum uniaxial strain vs. number of cycles, under fatigue loadings with maximum stress $\sigma_{11\text{max}}=0.94\sigma_0$ and $\sigma_{11\text{max}}=1.11\sigma_0$ applied at $0^\circ$ angle w.r.t. MFD.

The model captures the main experimental tends. However it underestimates the value of maximum strains especially under high level of applied stresses. This may be due to the self heating effect which is not taken into account in this model, as it is shown in figure 5.2.12 for maximum strains in $90^\circ$ direction. Indeed, the generated temperature during fatigue loading may induce a loss of material stiffness which may be the origin of further deformation within the material. Another reason may be the use of the average of orientation tensor over the specimen thickness in the MFH procedure.
5.2 Proposed modeling approach and its evaluation

Number of cycles

Normalized strain ($\frac{\sigma_{1\text{max}}}{\sigma_0}$)

EXP SIMU

Max strain $\sigma_{1\text{max}} = 0.47 \sigma_0$

Max strain $\sigma_{1\text{max}} = 0.58 \sigma_0$

Max strain $\sigma_{1\text{max}} = 0.64 \sigma_0$

Self-heating ($T_{\text{for} \: \sigma_{1\text{max}}} \text{[C]}$)

$\sigma_{1\text{max}} = 0.47 \sigma_0$

$\sigma_{1\text{max}} = 0.58 \sigma_0$

$\sigma_{1\text{max}} = 0.64 \sigma_0$

Figure 5.2.12: Experimental and numerical maximum uniaxial strain and the self-heating vs. number of cycles, under fatigue loadings with maximum stress $\sigma_{1\text{max}} = 0.47 \sigma_0$, $\sigma_{1\text{max}} = 0.58 \sigma_0$ and $\sigma_{1\text{max}} = 0.65 \sigma_0$ applied at 90° angle w.r.t. MFD.

In summary, the proposed model for predicting the macroscale behavior, consisting of a VE matrix and misaligned elastic inclusions, allows to obtain qualitatively good predictions that are representative of the material behavior in different case of loading corresponding to several angles w.r.t. MFD. Although the model predictions need to be improved, the obtained quantities such as matrix average strains, fibers average strains and the macro-strains, are useful in order to the evaluate the proposed fatigue model, as it is shown in the next subsection. Possible improvements of the model used for macroscale behavior are detailed in section 5.3.

5.2.2.3 Predictions of the material fatigue failure

This subsection is devoted to the study of the material lifetime, hence the focus here is on the behavior within the weak spots, which is assumed to obey to a damaged VEVP behavior. In order to estimate the external loading applied to the weak spots, the mean volumetric strain within the matrix and the macroscopic strain are tested in the following simulations. For each loading, the viscoplastic and damage parameters are identified by reverse engineering using one S-N curve chosen to be at 45°, the other S-N curves for orientation 0° and 90° are predicted. Note that the viscoelastic parameters of the weak spots are the same as those for the matrix material.

Using the matrix mean volumetric strain The first deformation applied to the weak spots is the mean volumetric strain within the matrix phase, since the weak spots are assumed to be part of the TP matrix. The S-N curve for direction 45° obtained by the experimental testing and the numerical simulation are showed in figure 5.2.13. The identified material parameters for the weak spots are listed in table 5.2.
5.2 Proposed modeling approach and its evaluation

Figure 5.2.13: Numerical and experimental S-N curves for dumbbell with cut-out angle equal to 45°, in the case of matrix mean volumetric strain as external loading applied to the WSs. Material parameters are listed in table 5.2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tr>
<td>Yield stress</td>
<td>( \sigma_y = 0.5 ) MPa</td>
</tr>
<tr>
<td>VP function</td>
<td>( \eta = 2.5 \times 10^{13} ) MPa.s ( m = 6 )</td>
</tr>
<tr>
<td>Damage parameters</td>
<td>( S = 0.2 ) MPa ( s = 2 ) ( Dc = 0.25 )</td>
</tr>
</tbody>
</table>

Table 5.2: Identified viscoplastic and damage parameters of the weak spots, in the case of matrix mean volumetric strain as external loading applied to the weak spots.

Once the material parameters are identified, the model predictions are compared to the experimental results under 0° and 90°. The numerical predictions are shown in figures 5.2.14 and 5.2.15. The model predictions for 0° are over estimated compared to the experimental results, whereas in the case of 90° the prediction underestimates the lifetime of the material. In order to try to explain the obtained results, the equivalent average strain within the matrix for different orientations w.r.t. MFD under maximum stresses corresponding to experimentally measured 10^4 cycles to failure, is plotted in figure 5.2.16. Although few cycles are not enough, in order to have an accurate evaluation of all the strain history during the loading, the magnitude of the equivalent strains may explain the damage evolution. Theoretically, the damage should be comparable in the case of the 3 angles, which is not the case as is shown in the figure 5.2.17.
5.2 Proposed modeling approach and its evaluation

Figure 5.2.14: Numerical and experimental S-N curves for dumbbell with cut-out angle equal to 0°, in the case of matrix mean volumetric strain as external loading applied to the weak spots. Material parameters are listed in table 5.2.

Figure 5.2.15: Numerical and experimental S-N curves for dumbbell with cut-out angle equal to 90°, in the case of matrix mean volumetric strain as external loading applied to the weak spots. Material parameters are listed in table 5.2.
5.2 Proposed modeling approach and its evaluation

Figure 5.2.16: The equivalent average strain within the matrix for different orientations w.r.t. MFD under maximum stresses corresponding to experimentally measured $10^4$ cycles to failure.

Figure 5.2.17: Effect of the orientation on the damage evolution within the weak spots, in the case of matrix mean volumetric strain as external loading applied to the weak spots.

Using the macro-strain  Here, the macro-strain is applied to the weak spots instead of the matrix volume average strain. Similar to previous case, the material parameters are identified based on the S-N curve for direction 45° (cf. figure 5.2.18). The identified material parameters for the weak spots are listed in table 5.3. The predictions for angles 0° and 90° are shown in figures 5.2.19 and 5.2.20, respectively. Employing the macro strain gives better predictions compared to those using the matrix strain.
5.2 Proposed modeling approach and its evaluation

Figure 5.2.18: Numerical and experimental S-N curves for dumbbell with cut-out angle equal to 45°, in the case of macro strain as external loading applied to the weak spots. Material parameters are listed in table 5.3.

<table>
<thead>
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<th>Value</th>
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</thead>
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<tr>
<td>Yield stress</td>
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</tr>
<tr>
<td>VP function $g_v$</td>
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<td>Damage parameters</td>
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</tr>
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<td>$s$</td>
<td>2</td>
</tr>
<tr>
<td>$D_c$</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Table 5.3: Identified viscoplastic and damage parameters of the weak-spots, in the case of macro strain applied as a external loading to the weak spots.

Similar to the previous analysis, the equivalent macro-strains are plotted in figure 5.2.21 for applied loading that should give $10^4$ cycles as lifetime of the dumbbells with different cut-out angles. The magnitude of the different equivalent strains seems to be closer, this is due to the contribution of the fibers strain (cf. figure 5.2.22). The evolution of the damage in the weak spots seems also to be closer, but it still different (cf. figure 5.2.23).
5.2 Proposed modeling approach and its evaluation

Figure 5.2.19: Numerical and experimental S-N curves for dumbbell with cut-out angle equal to 0°, in the case of macro strain as external loading applied to the weak spots. Material parameters are listed in table 5.3.

![Figure 5.2.19](image_url)

Figure 5.2.20: Numerical and experimental S-N curves for dumbbell with cut-out angle equal to 90°, in the case of macro strain as external loading applied to the weak spots. Material parameters are listed in table 5.3.

![Figure 5.2.20](image_url)
5.2 Proposed modeling approach and its evaluation

Figure 5.2.21: The equivalent macro-strain for different orientations w.r.t. MFD under maximum stresses corresponding to experimentally measured $10^4$ cycles to failure.

Figure 5.2.22: The equivalent average strain within the fibers for different orientations w.r.t. MFD under maximum stresses corresponding to experimentally measured $10^4$ cycles to failure.
5.3 Discussion and possible enhancements

**About material modeling**

In this work, the behavior of the matrix is assumed to be VE behavior. More complex material behavior may be considered in order to better capture the macroscale behavior such as the VEVP model or the VEVPD model with or without kinematic hardening. Also, considering the self heating generated during loading and its effect on the material behavior. This could be made by considering temperature-dependent material model for the matrix and the weak spots. Estimating self heating may be based on a part of dissipated energy which enters the heat equation as a source term.

In order to take into account the failure of the interface, *i.e.* the fiber matrix debonding, one can assume that the fibers together with the interface are modeled using one phase, which has a nonlinear damaged behavior: EPD, EVPD or VEVPD.

Considering a layered RVE with different orientation tensors and fiber concentration in each layer, may improve the macroscale prediction. The main challenge is to estimate the volume fraction in each layer and define the boundary conditions, since the applied load in each layer may be different, especially in the case of fatigue loading since the applied load is stress controlled.

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**Figure 5.2.23:** Effect of the orientation on the damage evolution within the weak spots, in the case of macro-strain as external loading applied to the weak spots.
5.4 Conclusion

The use of statistical second moments MFH techniques as the one proposed for E(V)P composites (Doghri et al., 2011) may improve predictions compared to the first order MFH method used in this work. MFH schemes with statistical second moments help to measure the variance and take into account the field fluctuations inside the phases with respect to the mean value. Hence, it may allow to better estimate the load applied to the weak spots.

**About fatigue failure modeling**  In order to estimate the fatigue failure of the material, an uncoupled approach was used in this work, based on the assumption of separating the macroscale behavior and fatigue behavior. The enhancements proposed for material modeling may improve the prediction of the fatigue failure. Especially, considering a layered RVE and applying the fatigue model using the concept of weak spots in each layer may give better predictions.

In order to better capture the effect of fiber orientation, an anisotropic damage may be considered within the weak spots and depending on the applied loading principal direction. Another possibility is to assume that the shape of the weak spots is spheroidal and oriented in the same direction of the fibers direction within the pseudo grain.

In the VEVPD model, a critical damage is used in order to capture the final failure of the material, another criterion may be proposed based on a critical value of the dissipated energy.

5.4 Conclusion

In this chapter, a literature review about the modeling of SFRTPs was presented, the majority of existing approaches are based on the crack initiation prediction. The proposed approach may also be classified as a crack initiation based approach since it neglect the crack propagation stage. The proposed method is based on MFH techniques and damage mechanics, in order to evaluate the macroscale behavior of the material during the fatigue loading and the fatigue failure behavior separately.

The different proposed models seem to reproduce the main experimental tendencies. Possible enhancements and a discussion were given in the last section.
Chapter 6

Conclusions and prospects

Throughout this thesis, we proposed several modeling approaches for the damage and failure of homogeneous and short-fiber reinforced thermoplastics under monotonic and fatigue loadings, motivated by experimental observations detailed in the introduction chapter. Mean-field homogenization techniques and continuum damage mechanics (CDM) are the main tools employed for the development of the proposed approaches.

A new constitutive model for viscoelastic-viscoplastic damaged (VEVPD) thermoplastic polymers was proposed. It was employed in order to simulate the behavior of several TPs mainly under monotonic loadings. It also correctly captures the unloading, reloading hysteresis loops for at least the first cycles.

A new MFH scheme based on the incrementally affine linearization method was proposed for two-phase VEVPD composites, where both the matrix and the inclusions obey the proposed VEVPD model.

For the HCF of TPs, we proposed a two-scale crack initiation based approach which neglects the crack propagation stages of the fatigue behavior. The volume where the fatigue failure may occur is assumed to be composed of a VE matrix which contains so-called weak spots representing preexisting defects and inhomogeneities within the material. The MFH scheme was used to predict the interaction between the weak spots assumed to be VEVPD and the matrix. The proposed model showed a good ability to predict the fatigue lifetime of unreinforced thermoplastics under multiaxial fatigue loadings. The mean stress effect was also successfully captured.

For the HCF of SFRTPs fatigue problem, a similar multiscale approach is proposed whereas the volume element where fatigue failure may happen, is composed of a VE matrix, misaligned fibers and VEVPD weak spots. The volume element may be seen as a three-phase composite. In order to simplify the problem, an uncoupled approach was privileged based on the assumption that the weak spots have negligible effect on the macroscale material behavior. By considering this assumption, the first problem is then equivalent to two uncoupled problems: a macroscale problem defined by a volume element composed of a VE matrix and misaligned elastic fibers, and a fatigue failure behavior problem defined by VEVPD weak spots.

The predictions of the model proposed for the macroscale problem, are com-
parable to the experimental results. The proposed approach may be more accurate by including into account self heating and a better description of the material microstructure, as it is detailed hereafter. The loading applied on the weak spots, is estimated based on evaluation of the average state in each phase of the macroscale problem: matrix and inclusion and the overall behavior. The macroscale strain and the matrix strain are used as loading applied to the weak spots. The different proposed modeling approaches seem to solve successfully the treated problems. However, in order to be improved and enlarge their validity domains, several proposals are given in the text, and they are summarized hereafter.

**Enhancement of the VEVPD model** Several directions are possible in order to enhance the VEVPD model and expand its range of validity. Hereafter a list of those directions:

  Extend the model to non-isothermal behavior: This is useful in order to model both the effect due to a thermal problem and also dissipation-induced self heating. Using the principal of time–temperature superposition for linear viscoelastic materials, the present formulation of VEVPD model may be extended to non-isothermal behavior. An attempt to apply this idea was proposed by Miled (2011) for his VEVP model (Miled et al., 2011).

  Model the self heating of the material: As shown in the text the effect seems to be important in some case of loading on the TPs based materials. Employing the dissipated energies estimation given by the model may allow to compute the energy converted into heat during loading. Then the self heating may contribute to irreversible loss of the material stiffness.

  The effect of hydrostatic pressure: Since the presented model is using the Von Mises yield criterion this phenomenon is not well taken into account, although the damage law is sensitive to the hydrostatic stress. To overcome this limitation a generalized Drucker-Prager criterion could be used, which will mainly involve important modifications to the numerical algorithm.

  Extend the model to large deformation: There is a work in progress within the research team about extending the VEVPD model to finite strain formulation. Instead of additive decomposition of total strain, the total deformation gradient is multiplicatively split into viscoelastic and viscoplastic parts.

**About the MFH of VEVPD composites** As explained in the discussion part of the chapter, the proposed MFH method based on incrementally affine linearization needs to be improved in order to eliminate the time increment sensitivity and the overestimation of the stiffness mainly in the nonlinear part of the composite behavior (cf. section 3.5 for more details).

In addition the use of MFH techniques with statistical second moments may lead to better predictions based on estimates of the variance and the field fluctuations inside the phases with respect to the mean (volume average values) as proposed for EVP composites by Doghri et al. (2011).
Enhancement of the HCF model for TPs  The proposed model showed good capabilities to capture the main effects observed experimentally, which are the mean stress effect and the sensitivity to multiaxial loading. However, some enhancement needs to be done in order to better capture these effects.

Possible enhancement in order to better capture the mean stress may be accomplished by using a different yield function which separates the viscoelastic and the viscoplastic behavior, similar to the proposal of Desmorat et al. (2015) for metals where the fatigue damaged zones assumed to obey to EP behavior.

For low cycle fatigue, defined by high frequency or high level of applied mechanical loading, a macroscale approach such as the Janssen et al. (2008b) approach is more suitable than the weak spots concepts. The proposed VEVPD model may be used at macroscale for this purpose, however, a modification is needed in order to take into account self-heating.

Enhancement of the HCF model for SRFTPs  Considering a layered volume element with different orientation tensor and fiber concentration in each layer, may improve the macroscale behavior prediction. The main challenge is to estimate the volume fraction in each layer and defining the boundary conditions, since the applied load in each layer may be different, especially in the case of fatigue loading since the applied load is stress controlled.

The use of statistical second moments MFH techniques as the one proposed for E(V)P composites Doghri et al. (2011) may improve predictions compared to the first order MFH method used in this work. Hence, it may allow to better estimate the load applied to the weak spots.

In this work, the behavior of the matrix is assumed to be VE behavior. More complex material behavior may be considered in order to better capture the macroscale behavior such as the VEPD model or the VEVPD model with or without kinematic hardening. Also, considering the self-heating generated during loading and its effect on the material behavior. This could be made by considering temperature-dependent material model for the matrix and the weak spots and estimating self-heating based on a part of dissipated energy which enters the heat equation as a source term.

In order to take into account the failure of the interface, i.e., the fiber-matrix debonding, one can assume that the fibers together with the interface are modeled using one phase, which has a nonlinear damaged behavior: EPD, EVPD or VEVPD.

In order to estimate the fatigue failure of the material, an uncoupled approach was used in this work, based on the assumption of separating the macroscale behavior and fatigue behavior. The enhancements proposed for material modeling may improve the prediction of the fatigue failure. Especially, considering a layered RVE and applying the fatigue model using the concept of weak spots in each layer may give better predictions.

In order to better capture the effect of fiber orientation, an anisotropic damage may be considered within the weak spots and depending on the applied loading principal direction. Another possibility is to assume that the shape of the weak spots is spheroidal and oriented in the same direction of the fiber direction within the pseudo grain.
About computation time  The main advantages of using MFH compared to full computation is CPU time consuming. But, this advantage needs be improved, especially in the case of HCF loadings. The computation time is one of the major limitations of the material model approaches applied to fatigue of materials, thus a method such as homogenization in time method proposed by Haouala and Doghri (2015) for VEVp materials is needed in order to allow industrial application of this kind of models. The work of Haouala and Doghri may be extended to the developed models and help to limit the time of computation.
Appendix A

Constitutive relations for the VEVPD model

A.1 Thermodynamical derivation of constitutive relations

Similarly to (Christensen, 1982) in linear viscoelasticity, for the proposed viscoelastic-viscoplastic model coupled with damage, the expression of $\rho \psi^{ve}$ is written as:

$$\rho \psi^{ve}(t) = (1 - D(t))Y(t)$$  \hspace{1cm} (A.1.1)

Where $Y(t)$ is defined as:

$$Y(t) = \frac{1}{2} \int_{-\infty}^{t} \int_{-\infty}^{t} \frac{\partial \varepsilon^{ve}(\tau)}{\partial \tau} : C^{ve}(t - \tau, t - \eta) : \frac{\partial \varepsilon^{ve}(\eta)}{\partial \eta} d\tau d\eta$$  \hspace{1cm} (A.1.2)

Similarly to elasto-viscoplasticity, Helmholtz free energy function $\psi$ is:

$$\rho \psi(t) = \rho \psi^{ve}(t) + \frac{a}{2} \alpha(t) : \alpha(t) + \int_{0}^{\tau(t)} R(\xi) d\xi$$  \hspace{1cm} (A.1.3)

Then the total derivative of $\rho \psi(t)$ with respect to $t$ is expressed as:

$$\rho \frac{d\psi(t)}{dt} = (1 - D) \frac{dY(t)}{dt} - Y(t) \frac{dD(t)}{dt} + a \alpha(t) : \frac{d\alpha(t)}{dt} + R(t) \frac{dr(t)}{dt}$$  \hspace{1cm} (A.1.4)

Using the Leibniz rule, the symmetry $C^{ve}_{ijkl}(\tau, \eta) = C^{ve}_{klij}(\eta, \tau)$ and the particular form $C^{ve}(\tau, \eta) = C^{ve}(\tau + \eta)$, the total derivative of $Y(t)$ with respect to $t$ is as follows:
A.1 Thermodynamical derivation of constitutive relations

\[
\frac{dY(t)}{dt} = \frac{1}{2} \int_{-\infty}^{t} \int_{\tau}^{t} \partial \varepsilon^{ve}(\tau) : \partial C^{ve}(2t-\tau-\eta) \cdot \partial \varepsilon^{ve}(\eta) \cdot d\tau d\eta \\
+ \left\{ \int_{-\infty}^{t} C^{ve}(t-\tau) : \partial \varepsilon^{ve}(\tau) \cdot d\tau \right\} : \partial \varepsilon^{ve}(t) \cdot \frac{\partial C^{ve}}{\partial t}
\]

(A.1.5)

Then using equation (A.1.4) the expression of \( \frac{d\psi}{dt} \) is found as:

\[
\rho \frac{d\psi}{dt} = (1 - D) \left\{ \int_{-\infty}^{t} C^{ve}(t-\tau) : \partial \varepsilon^{ve}(\tau) \cdot d\tau \right\} : \partial \varepsilon^{ve}(t) \\
+ (1 - D) \frac{1}{2} \int_{-\infty}^{t} \int_{\tau}^{t} \partial \varepsilon^{ve}(\tau) : \partial C^{ve}(2t-\tau-\eta) \cdot \partial \varepsilon^{ve}(\eta) \cdot d\tau d\eta \\
- Y(t) \frac{dD(t)}{dt} + a\alpha(t) : \frac{d\alpha(t)}{dt} + R(r) \frac{dr(t)}{dt}
\]

(A.1.6)

On the following, due to the hypothesis of small perturbation \( \frac{d\varepsilon^{ve}}{dt} = \frac{\partial \varepsilon^{ve}}{\partial t} \)

and similarly to Christensen (1982), the expression of the Cauchy stress is found using the inequality of Clausius-Duhem which requires the dissipation to be non-negative

\[
\phi = \sigma : \dot{\varepsilon}^{ve} - \rho \frac{d\psi}{dt} \geq 0
\]

(A.1.7)

then

\[
\phi = \left( \sigma - (1 - D) \int_{-\infty}^{t} C^{ve}(t-\tau) : \partial \varepsilon^{ve}(\tau) \cdot d\tau \right) : \dot{\varepsilon}^{ve}(t) + \sigma : \dot{\varepsilon}^{vp}(t) \\
-(1 - D) \frac{1}{2} \int_{-\infty}^{t} \int_{\tau}^{t} \partial \varepsilon^{ve}(\tau) : \partial C^{ve}(2t-\tau-\eta) \cdot \partial \varepsilon^{ve}(\eta) \cdot d\tau d\eta \\
+ Y \dot{D} - a\alpha : \dot{\alpha} - R\dot{r} \geq 0
\]

(A.1.8)

Where a superposed dot designates a total time derivative. The inequality must hold for all arbitrary values of the derivative \( \dot{\varepsilon}^{ve} \), therefore, its coefficient should vanish. Hence,

\[
\sigma(t) = (1 - D(t)) \int_{-\infty}^{t} C^{ve}(t-\tau) : \partial \varepsilon^{ve}(\tau) \cdot d\tau
\]

(A.1.9)

The dissipation is then

\[
\phi = \sigma : \dot{\varepsilon}^{vp} + (1 - D)\phi^{ve} + Y \dot{D} - a\alpha(t) : \dot{\alpha} - R\dot{r} \geq 0
\]

(A.1.10)
A.2 Expressions of the damage thermodynamic force and the VE dissipation using Prony series

where:

\[ \phi^{ve}(t) = -\frac{1}{2} \int_{-\infty}^{t} \int_{-\infty}^{\tau} \partial \xi^{ve}(\tau) \partial \xi^{ve}(\eta) \partial \xi^{ve}(\eta) \partial \eta \ d\tau d\eta \quad (A.1.11) \]

A.2 Expressions of the damage thermodynamic force and the VE dissipation using Prony series

The damage thermodynamic force (eq. A.1.2) is rewritten, using equations (eq. 2.2.15) and (eq. 2.2.19), as:

\[ Y(t) = \int_{-\infty}^{t} \int_{-\infty}^{t} \left( G(2t - \tau - \eta) \frac{\partial \xi^{ve}(\tau)}{\partial \tau} \frac{\partial \xi^{ve}(\eta)}{\partial \eta} \right) d\tau d\eta \]

\[ + \frac{9}{2} \int_{-\infty}^{t} \int_{-\infty}^{t} \left( \frac{K(2t - \tau - \eta)}{g_i} \frac{\partial \xi^{ve}(\tau)}{\partial \tau} \frac{\partial \xi^{ve}(\eta)}{\partial \eta} \right) d\tau d\eta \quad (A.2.1) \]

On the other hand, the use of Prony series (eq. 2.2.16) leads to:

\[ Y^d(t) = G_\infty \xi^{ve}(t) : \xi^{ve}(t) \]

\[ + \sum_{i=1}^{l} G_i \int_{-\infty}^{t} \int_{-\infty}^{t} \exp \left( \frac{\tau - t}{g_i} \right) \exp \left( \frac{\eta - t}{g_i} \right) \frac{\partial \xi^{ve}(\eta)}{\partial \eta} \frac{\partial \xi^{ve}(\tau)}{\partial \tau} d\tau d\eta \]

\[ Y_{H}(t) = \frac{9}{2} K_\infty \left( \xi^{ve}(t) \right)^2 \]

\[ + \sum_{j=1}^{\infty} \frac{9}{2} K_j \int_{-\infty}^{t} \int_{-\infty}^{t} \exp \left( \frac{\tau - t}{k_j} \right) \exp \left( \frac{\eta - t}{k_j} \right) \frac{\partial \xi^{ve}(\tau)}{\partial \tau} \frac{\partial \xi^{ve}(\eta)}{\partial \eta} d\tau d\eta \quad (A.2.2) \]

Then, using equations (eq. 2.2.17;eq. 2.2.18), we obtain:

\[ Y = \frac{s_{\infty}}{4G_{\infty}} + \left( \frac{\hat{\sigma}_{H_{\infty}}}{2K_{\infty}} \right)^2 + \sum_{i=1}^{l} \frac{\hat{s}_{i}(t)}{4G_{i}} + \sum_{j=1}^{\infty} \frac{\left( \hat{\sigma}_{H_{j}}(t) \right)^2}{2K_{j}} \quad (A.2.3) \]

Since the VE dissipation (eq. A.1.11) is similar to the expression of the energy release rate Y (eq. A.1.2), its expression is computed similarly using Prony series and found to be:

\[ \phi^{ve} = \sum_{i=1}^{l} \frac{\hat{s}_{i}}{4G_{i}g_i} + \sum_{j=1}^{\infty} \frac{\left( \hat{\sigma}_{H_{j}} \right)^2}{2K_{j}k_{j}} \quad (A.2.4) \]
Appendix B

Numerical algorithm for the VEVPD model

B.1 Radial return algorithm

The numerical algorithm was developed following the methods developed in (Doghri, 1993, 1995; Simo and Hughes, 1998; Miled et al., 2011), based on a strain-driven procedure. This algorithm should compute the variables at time $t_{n+1}$. $\Delta(\bullet) = (\bullet)_{n+1} - (\bullet)_n$ designates an increment over a generic time interval $[t_n, t_{n+1}]$.

B.1.1 Viscoelastic predictor

The first step in the proposed return mapping algorithm is called “viscoelastic predictor”, assuming that the increment is entirely viscoelastic ($\Delta e^{ve} = \Delta e$ and $\Delta e^{vp} = 0$). The effective trial stress is given by

$$\mathbf{\tilde{\sigma}}^{tr}(t_{n+1}) = C^{ve}_\infty : \mathbf{e}^{ve}(t_n) + \mathbf{\tilde{C}}^{ve} : \Delta \mathbf{e} + \sum_{i=1}^{l} \exp(-\frac{\Delta t}{g_i}) \mathbf{\tilde{s}}_i(t_n)$$

$$+ \sum_{j=1}^{j} \exp(-\frac{\Delta t}{k_j}) \mathbf{\tilde{\sigma}}_{H_j}(t_n) I$$

(B.1.1)

with

$$C^{ve}_\infty = 2G^{\text{dev}}_\infty + 3K^{\text{vol}}_\infty$$

(B.1.2)

$$\begin{cases} \mathbf{\tilde{s}}_i(t_{n+1}) = 2G_i \left[ 1 - \exp\left(-\frac{\Delta t}{g_i}\right) \right] \frac{g_i}{\Delta t} \Delta \mathbf{e}^{ve} + \exp\left(-\frac{\Delta t}{g_i}\right) \mathbf{\tilde{s}}_i(t_n) \\ \mathbf{\tilde{\sigma}}_{H_j}(t_{n+1}) = 3K_j \left[ 1 - \exp\left(-\frac{\Delta t}{k_j}\right) \right] \frac{k_j}{\Delta t} \Delta \mathbf{e}^{ve} + \exp\left(-\frac{\Delta t}{k_j}\right) \mathbf{\tilde{\sigma}}_{H_j}(t_n) \end{cases}$$

(B.1.3)

which leads to:
B.1 Radial return algorithm

\[ \Delta \bar{\sigma} = \ddot{\sigma}^{ve}(\Delta t) : \Delta \bar{\epsilon} + a(t_n) \]  

(B.1.4)

where: \( \ddot{\sigma}^{ve} = 2\dot{G}^{dev} + 3\dot{K}^{vol} \); \( \dot{G} \) and \( \dot{K} \) are defined as follows:

\[
\begin{align*}
\dot{G} &= G_\infty + \sum_{i=1}^I G_i \dot{G}_i(\Delta t) \quad \text{with} \quad \dot{G}_i(\Delta t) = \left[ 1 - \exp\left( -\frac{\Delta t}{g_i} \right) \right] \frac{g_i}{\Delta t} \\
\dot{K} &= K_\infty + \sum_{j=1}^J K_j \dot{K}_j(\Delta t) \quad \text{with} \quad \dot{K}_j(\Delta t) = \left[ 1 - \exp\left( -\frac{\Delta t}{k_j} \right) \right] \frac{k_j}{\Delta t}
\end{align*}
\]

and

\[
a(t_n) = -\sum_{i=1}^I \left[ 1 - \exp\left( -\frac{\Delta t}{g_i} \right) \right] \bar{s}_i(t_n) - \sum_{j=1}^J \left[ 1 - \exp\left( -\frac{\Delta t}{k_j} \right) \right] \bar{s}_v(t_n)I
\]

(B.1.5)

and the trial stress is then:

\[
\bar{\sigma}^{tr}(t_{n+1}) = (1 - D_n) \bar{\sigma}^{tr}(t_n) + a(t_n)
\]

(B.1.6)

If the trial effective stress satisfies the yield condition:

\[
f^{tr} = (\bar{\sigma}^{tr}_n - X_n)_{eq} - \sigma_y - R(r_n) \leq 0
\]

(B.1.7)

Then the viscoelastic predictor is indeed the solution at \( t_{n+1} \):

\[
\bar{s}_{n+1} = \bar{s}_{n+1}^{te}; \quad D_{n+1} = D_n; \quad \bar{e}_{n+1}^{tr} = \bar{e}_{n+1}^{tr}; \quad \text{and} \quad \bar{e}_{n+1}^{vp} = \bar{e}_{n+1}^{vp}
\]

Otherwise, viscoplastic strains have changed during the time interval and a "viscoplastic corrector" is needed. The unknown effective stress at \( t_{n+1} \) could be expressed as following:

\[
\bar{s}_{n+1} = \bar{s}_{n+1}^{tr} - \dot{\sigma}^{ve} : \Delta \bar{e}^{vp}
\]

(B.1.9)

Since \( \Delta \bar{e}^{vp} \) is deviatoric, then \( tr(\bar{s}_{n+1}) = tr(\bar{s}_{n+1}^{tr}) \). Which gives that \( \bar{s} = \bar{s}^{tr} - 2\dot{G}\Delta \bar{e}^{vp} \) with \( \bar{s} \) is the deviatoric effective stress.

\[ \text{B.1.2 Correction over viscoelastic predictor} \]

Time discretization of constitutive equations (2.2.33) using the backward Euler scheme gives the following set of equations:

\[
\bar{s} = \bar{s}^{tr} - 2\dot{G}\Delta \bar{e}^{vp}
\]

(B.1.10)

\[
f = (\bar{s} - X)_{eq} - \sigma_y - R(r)
\]

\[
\Delta \bar{e}^{vp} = \bar{N} \Delta p
\]

\[
\Delta X = (1 - D)(a \Delta \bar{e}^{vp} - bX \Delta p)
\]

\[
\Delta D = y \Delta p
\]

\[
\Delta r = (1 - D) \Delta p
\]

\[
\Delta r = g_v ((\bar{s} - X)_{eq}, r) \Delta t
\]
B.1 Radial return algorithm

where

\[ y = \left( \frac{Y}{S} \right)^{s} \quad \text{with} \quad Y = \frac{\tilde{s}_{\infty}^{2} - \tilde{s}_{\infty}^{2}}{4G_{\infty}} + \frac{\left( \tilde{H}_{L} \right)^{2}}{2K_{\infty}} + \sum_{i=1}^{f} \frac{\tilde{s}_{i} - \tilde{s}_{i}}{4G_{i}} + \sum_{j=1}^{f} \frac{\left( \tilde{H}_{L} \right)^{2}}{2K_{j}} \]  

(B.1.11)

The problem is reduced to finding the four unknowns \( \tilde{s}, r, X \) and \( D \) which satisfy the following system of equations

\[
\begin{align*}
    k_{\tilde{s}} &= \tilde{s} - \tilde{s}_{tr} + 2\tilde{G}\tilde{N} \cdot \frac{\Delta r}{1 - D} = 0 \\
    k_{r} &= \Delta r - g_{c} ((\tilde{\sigma} - X)_{eq}, r) \Delta t = 0 \\
    k_{X} &= \Delta X - (a\tilde{N} - bX_{n}) \cdot \frac{\Delta r}{1 + b\Delta r} = 0 \\
    k_{D} &= \Delta D - y(\tilde{s}) \cdot \frac{\Delta r}{1 - D} = 0
\end{align*}
\]  

(B.1.12)

The following notations are introduced for convenience:

\[
h_{g,(\sigma,x)} = \frac{\partial g_{c}}{\partial (\tilde{\sigma} - X)_{eq}} \Delta t \\
h_{g,r} = \frac{\partial g_{c}}{\partial r} \Delta t
\]

Following the same procedure as proposed by Doghri (1995), for each iteration the expressions of iterative corrections \( (c_{a}) = (\bullet)^{(i+1)} - (\bullet)^{(it)} \) is obtained. The corrections obey to the following equations:

- The expression of \((c_{\tilde{s}} - c_{X})\) is given by:

\[
(c_{\tilde{s}} - c_{X}) = \frac{-1}{1 + (3/2)g} \left[ k_{\tilde{s}} - k_{X} + g\tilde{N} : (k_{\tilde{s}} - k_{X}) \tilde{N} \right] - \left[ 2\tilde{G}c_{p} + \frac{a}{(1 + b\Delta r)^{2}} \right] c_{r} \\
+ \frac{1}{1 + (3/2)g} \frac{b}{(1 + b\Delta r)^{2}} \left[ X_{n} + g(N : X_{n}) \tilde{N} \right] c_{r}
\]

(B.1.13)

where: \( g = \frac{1}{(\tilde{\sigma} - X)_{eq}} \left( 2\tilde{G}\Delta p + \frac{a\Delta r}{1 + (3/2)g} \right) \)

- The expression of \( c_{\tilde{s}} \) as a function of \( c_{r} \) and \( c_{p} \) is found as:

\[
c_{\tilde{s}} = -k_{\tilde{s}} - 2\tilde{G}\tilde{N}c_{p} + \frac{3\tilde{G}}{(\tilde{\sigma} - X)_{eq}} \frac{\Delta p}{1 + (3/2)g} \{ \ldots \} \]

(B.1.14)

- The expression of \( c_{D} \) as a function of \( c_{r} \) and \( c_{p} \) is found as:

\[
c_{D} = -k_{D} + y_{c} + (\Delta p) \frac{\partial y_{c}}{\partial \tilde{s}} \left[ -k_{\tilde{s}} - 2\tilde{G}\tilde{N}c_{p} + \frac{3\tilde{G}}{(\tilde{\sigma} - X)_{eq}} \frac{\Delta p}{1 + (3/2)g} \{ \ldots \} \right]
\]

(B.1.15)

In both (B.1.14, B.1.15), the expression between bracket is:

\[
\{ \ldots \} = k_{\tilde{s}} - k_{X} - 2\tilde{G}\tilde{N} : (k_{\tilde{s}} - k_{X}) \tilde{N} - \frac{b}{(1 + b\Delta r)^{2}} \left[ X_{n} - \frac{2}{3} (\tilde{N} : X_{n}) \tilde{N} \right] c_{r}
\]

(B.1.16)
B.1 Radial return algorithm

- The expression of $c_p$ as function of $c_r$ is found as:

$$c_p = -\frac{1}{3G} \left\{ \frac{k_r}{h_{g,(s,X)}} + \bar{N} : [k\bar{z} - kX] + \left[ \frac{1 - h_{g,r}}{h_{g,(s,X)}} + \frac{\frac{3}{2}a - b(\bar{N} : X_n)}{(1 + b\Delta r)^2} \right] c_r \right\}$$  

\[(B.1.17)\]

- And the expression of $c_r$ is:

$$c_r = \frac{\mathcal{N}}{h_{alg}}$$  

\[(B.1.18)\]

The numerator is given by the following expression:

$$\mathcal{N} = - \left[ (1 - D) - y\Delta p + 2\bar{G}(\Delta p)^2 \frac{\partial y}{\partial \bar{s}} : \bar{N} \right] \left\{ \frac{k_r}{h_{g,(s,X)}} + \bar{N} : [k\bar{z} - kX] \right\} + 3\bar{G}\Delta p \left[ k_D + (\Delta p) \frac{\partial y}{\partial \bar{s}} : k_i \right] - 3\bar{G}(\Delta p)^2 \frac{3\bar{G}}{(\bar{\sigma} - X)_{eq}}$$  

\[(B.1.19)\]

The denominator of $c_r$ is given by the following expression:

$$h_{alg} = 3\bar{G} + \left[ (1 - D) - y\Delta p + 2\bar{G}(\Delta p)^2 \frac{\partial y}{\partial \bar{s}} : \bar{N} \right]$$  

\[(B.1.20)\]

B.1.3 Summary of the numerical algorithm

The time-integration algorithm based on a strain-driven procedure, can be summarized as follows:
B.1 Radial return algorithm

Input: $\Delta x$ and $\Delta t$

Previous time step

Viscoelastic predictor

Compute $\tilde{\sigma}^r$ and $\sigma^r$ from Eqs. (B.1.1, B.1.6)

Update/initialize solution at $t_{n+1}$

$(\sigma, r, X, p, D) = (\sigma^r, r_n, X_n, p_n, D_n)$

$f^{tr} > 0$

Compute corrections $c_{(\bullet)}$:
- $c_r$ from Eq. B.1.18
- $c_p$ from Eq. B.1.17
- $c_t$ from Eq. B.1.14
- $(c_i - c_X)$ from Eq. B.1.13
- $c_X = c_t - (c_i - c_X)$
- $c_D$ from Eq. B.1.15

Update variables: $(\bullet) \leftarrow (\bullet) + c_{(\bullet)}$

Compute residuals from Eqs. (B.1.12)

Tolerance criteria satisfied?

no

$f^{tr} \leq 0$

yes

Next time step

Figure B.1.1: Numerical algorithm for the VEVPD material behavior
B.2 Consistent tangent operator

When the algorithm has converged, the corresponding consistent operator $C^{\text{alg}}$ is determined also by following the same procedure as in Doghri (1995). For the visco-elastic increment $C^{\text{alg}} = (1 - D_n)C^{\text{ve}}$, otherwise $C^{\text{alg}}$ is expressed as follows:

$$C^{\text{alg}} = (1 - D) \tilde{C}^{\text{alg}} - \tilde{\sigma} \otimes \left\{ (\Delta p)\tilde{C}^{\text{alg}} : \frac{\partial y}{\partial s} + \frac{2}{3} y \tilde{N} \right\}$$  \hfill (B.2.1)$$

where $\tilde{C}^{\text{alg}}$ is the effective tangent operator defined as:

$$\tilde{C}^{\text{alg}} = C^{\text{ve}} - \frac{(2\tilde{G})^2}{(\tilde{\sigma} - X)_{eq}} \frac{\Delta p}{1 + (3/2)g} \left( \frac{3}{2} I_{\text{dev}} - \tilde{N} \otimes \tilde{N} \right) - \frac{2}{3} \tilde{N} \otimes \left( 2\tilde{G} \tilde{N} \right)$$  \hfill (B.2.2)

and

$$n^{\text{alg}} = \left[ (1 - D) - y \Delta p + 2\tilde{G}(\Delta p)^2 \frac{\partial y}{\partial s} : \tilde{N} \right] 2\tilde{G} \tilde{N}$$  \hfill (B.2.3)
Appendix C

Identification procedure of dynamic properties of linear viscoelastic materials

Properties of real materials can be assessed based on dynamic experiments which can be conducted in stress-or strain controlled modes of deformation. A harmonic oscillation is applied in a wide frequency range under small strain and we measure the resulting stress. In order to represent mathematically these harmonic oscillations, it is convenient to use complex numbers. For the deformation-controlled experiment, the strain and stress can be expressed as follows:

\[ \varepsilon(t) = \varepsilon_0 \exp(iwt), \quad \sigma(t) = f(\varepsilon(t)) \quad (C.0.1) \]

where \( \varepsilon_0 \) is the amplitude of deformation of the harmonic oscillation and \( w \) is the frequency. The dynamic modulus is the ratio of stress to strain \( E^*(iw) = \frac{\sigma(t)}{\varepsilon(t)} \) and is a material property. Using the response to a steady-state sinusoidal loading, \( E^*(iw) \) can be written as a sum:

\[ E^*(iw) = E'(w) + iE''(w) \quad (C.0.2) \]

where the real part \( E'(w) \) is defined as the storage modulus (which measures the stored energy, representing the elastic portion) and the imaginary part \( E''(w) \) is defined as the loss modulus (it measures the energy dissipated as heat, representing the viscous portion). We can also write the relaxation modulus in the time domain as a Prony series:

\[ E(t) = E_\infty + \sum_{(i)} E_i \exp \left( -\frac{t}{\tau_i} \right) \quad (C.0.3) \]

Using Laplace transform, we can write:

\[ \text{This appendix is taken from Miled (2011)} \]
\[ L_c \{ E(t) \} = E^* (s) = E_\infty + \sum_{i} \frac{E_i s}{s + \frac{1}{\tau_i}} \]  
(C.0.4)

where \( E^*(s) \) is the relaxation modulus in the Laplace domain. If we take \( s = iw \), the previous equation becomes:

\[ E^* (iw) = E_\infty + \sum_{i} \frac{E_i w^2}{\left( \frac{1}{\tau_i} \right)^2 + w^2} + i \sum_{i} \frac{E_i w}{\left( \frac{1}{\tau_i} \right)^2 + w^2} \]  
(C.0.5)

Real part: \( E'(w) \)

Imaginary part: \( E''(w) \)
Appendix D

Tsai-Hill criterion

The Tsai-Hill criterion (Tsai and Wu, 1971) is considered to be an adaptation of the Von Mises criterion. Based on the work of Hill on yielding and plastic flow of anisotropic metals (Hill, 1948). The classical Tsai-Hill criterion for static strength of anisotropic materials is generally written as:

\[ H (\sigma_{11} - \sigma_{22})^2 + F (\sigma_{22} - \sigma_{33})^2 + G (\sigma_{33} - \sigma_{11})^2 + N\sigma_{12}^2 + P\sigma_{13}^2 + Q\sigma_{23}^2 = 1 \]  \hspace{1cm} (D.0.1)

where \( H, F, G, N, P \) and \( Q \) are material parameters. The criterion can be also expressed in tonsorial form using using a fourth order tensor \( M \):

\[
\sigma : M : \sigma = 1 \quad \text{(D.0.2)}
\]

with is defined by a \( 6 \times 6 \) matrix as:

\[
\mathbf{M} = \begin{bmatrix}
G + H & -G & -H & 0 & 0 & 0 \\
F + H & -F & 0 & 0 & 0 & 0 \\
F + G & 0 & 0 & 0 & 0 & 0 \\
2N & 0 & 0 & 0 & 0 & 0 \\
sym & 2P & 0 & 0 & 0 & 0 \\
2Q & 0 & 0 & 0 & 0 & 0
\end{bmatrix} \quad \text{(D.0.3)}
\]

For unidirectional composites, the stress component \( \sigma_{ij} \), \( (i = 1..3) \) are equal to zero, then the equation D.0.1, will have the following expression:

\[
\left( \frac{\sigma_{11}}{\sigma_{\text{longi}}} \right)^2 + \left( \frac{\sigma_{22}}{\sigma_{\text{transv}}} \right)^2 - \frac{\sigma_{11}\sigma_{22}}{\sigma_{\text{longi}}^2} + 2 \left( \frac{\sigma_{12}}{\tau_{\text{longi}}} \right)^2 = 1 \]  \hspace{1cm} (D.0.4)

where:

\[
\sigma_{\text{longi}}^2 = \frac{1}{G + H} = \frac{1}{2G}; \quad \sigma_{\text{transv}}^2 = \frac{1}{F + H}; \quad \tau_{\text{longi}}^2 = \frac{1}{N}
\]
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